DualSPHysics Users Workshop 2016
Welcome

Benedict D. Rogers

School of Mechanical, Aerospace & Civil Engineering (MACE), University of Manchester

Welcome!

We warmly welcome you to the School of Mechanical, Aerospace and Civil Engineering at the University of Manchester

But first **some history**:

Manchester emerged as the **world's first industrial city**.

Manchester businessmen and industrialists established the **Mechanics' Institute** (Owen's College, UMIST, modern University of Manchester) to ensure their workers could learn the basic principles of science.

University can count **25 Nobel Prize winners** amongst its current and former staff and students

Manchester History

You are in a very historic place
for science & engineering!

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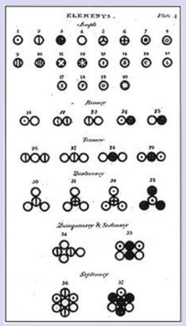
Role of Manchester in Scientific & Engineering Development

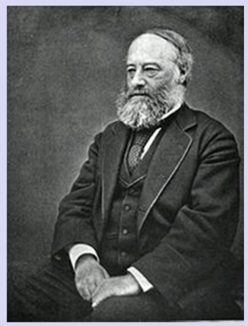
MODERN CHEMISTRY:

John Dalton (1766 – 1844) foundation of modern atomic theory



1st LAW THERMODYNAMICS

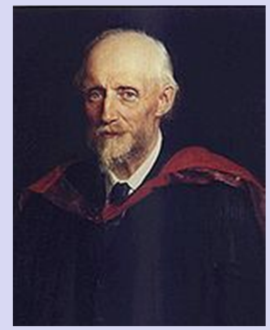
mechanical equivalence of heat postulated by **James Prescott Joule** (1819-89)



$$dU = \delta Q - \delta W$$

REYNOLDS NUMBER IN TURBULENT FLOWS:

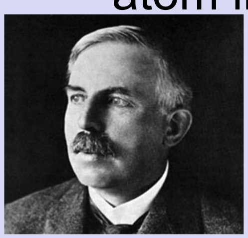
Experiments conducted by **Osborne Reynolds** the dimensionless number

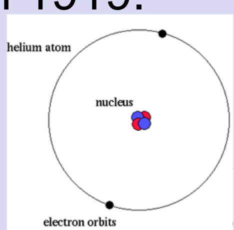


$$\mathrm{Re} = \frac{\rho V L}{\mu} = \frac{V L}{\nu}$$

SPLITTING THE ATOM

Ernest Rutherford at Manchester University discovered how to split the atom in 1919.

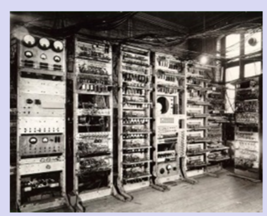




COMPUTERS

1st memory programmable computer &

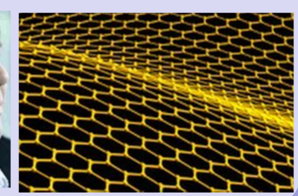
Alan Turing



GRAPHENE:

Thinnest supermaterial in the world

Won the Nobel Prize for Physics in 2010



Role of Manchester in Scientific & Engineering Development

Jodrell Bank (Cheshire) a Lovell built world's largest steerable radio telescope just after the Second World War.

Contraceptive pill (1961) and **first test tube baby** (IVF) was (1978).

World's 1st steam-powered mill, opened in 1783 by **Richard Arkwright** for cotton.

The **world's first railway station**

(Liverpool Road, 1830)

VOTES FOR WOMEN:

Pankhurst founded

Women's Social & Political Union in 1903

leading to the Suffragette Movement

World's 1st professional football league

set up in

1888 in the

Royal Hotel,

Manchester

School of MACE

What happens in MACE?

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School of Mechanical, Aerospace and Civil Engineering (MACE)

- **1000 Undergraduate students** on 3 programmes: Mech, Aero & Civil
- **1000 Postgraduate Taught (PGT) Students**
- **250 Postgraduate Research (PGR) Students**
- **120 Academic Staff + 60 Postdocs**

Laser manufacturing

Research in MACE:

- Aerospace engineering
- Bio-engineering
- Climate change
- Innovative manufacturing
- Management of projects
- Modelling and simulation
- Nuclear engineering
- Offshore energy and coastal engineering
- Structural and fire engineering

http://www.mace.manchester.ac.uk

Modelling and Simulation Centre (MaSC)

What happens in MACE?

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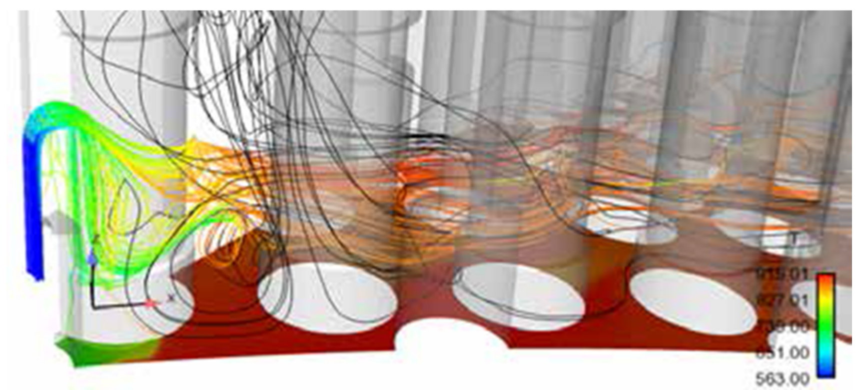
Modelling and Simulation Centre (MaSC)

- **EDF & University of Manchester** – established in 2011 a new centre focusing on M&S
- **Initially** CFD & Computational Solid Mechanics
- **Now includes** welding technology, long-term structural graphite integrity

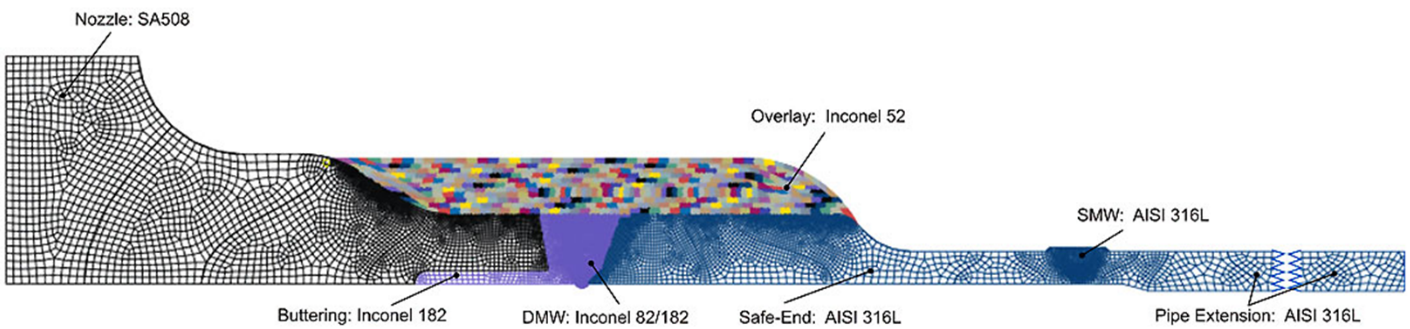
Aims of MaSC:

- **Scientific Excellence** – facilitating world-wide take-up of EDF open-source codes
- **Advanced Studies –** real engineering problems
- **Partnership** - stakeholders
- **Skills development** - training



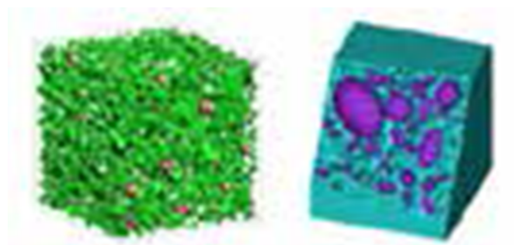
Modelling and Simulation Centre (MaSC)

Welding Technology– experimental and numerical investigations of microstructure & weld performance



Mechanics and Physics of Solids – quasi brittle materials, metallic materials, transport through porous media

Meso-scale modelling of conrete



Moisture in cement

Cracked graphite moderator

Modelling and Simulation Centre (MaSC)

And of course SPH!!!

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Overview

- Motivation and why SPH
- What is Smoothed Particle Hydrodynamics (**SPH**)?
- What can SPH do? Why is it revolutionising areas of engineering simulation?

- DualSPHysics
  - Where did it come from?
  - What is a GPU?
  - What can it do?
  - Who are the DualSPHysics team?
  - What SPH activity happens in Manchester

SPHERIC - SPH European Research Interest Community

Original Motivation for SPH

- **Free-surface flows** are rarely singly connected, e.g. beaches & wave energy devices

Breaking waves on beaches

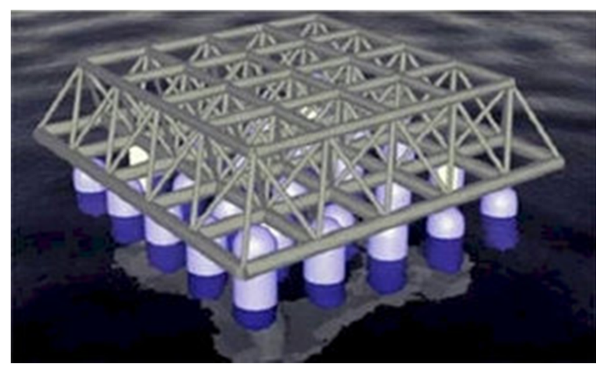
Plunger

Splash up

(Photo courtesy of F. Raichlen)

Overtopping:

Wave Energy Devices: Manchester Bobber

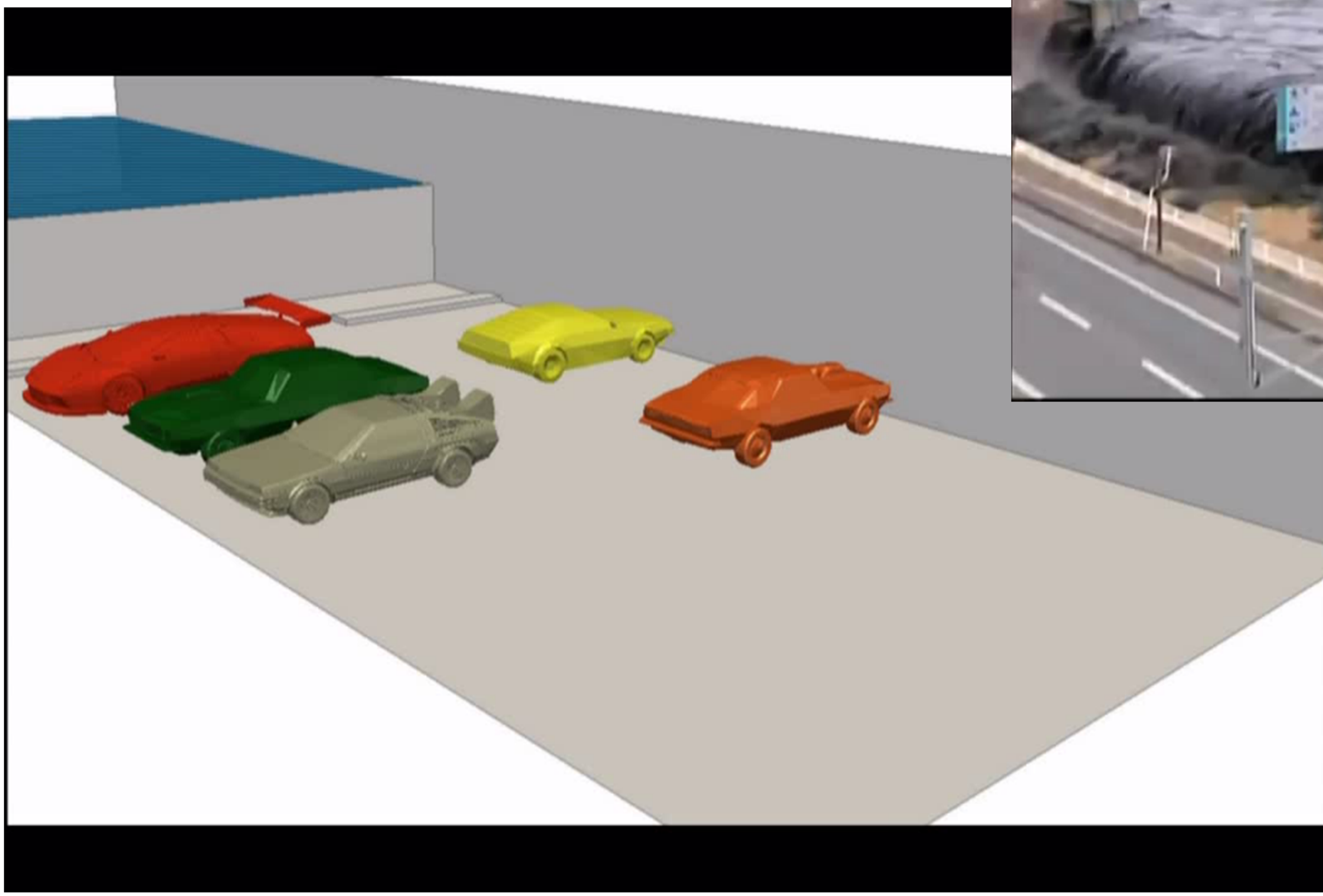


Very complex Multi-phase Multiscale problems

SPH: Has some distinct advantages in simulating these situations

Classical SPH Formulation Example

2011 Japanese Tsunami



Crespo et al. (2012)

Meshless methods: Basic Idea of SPH

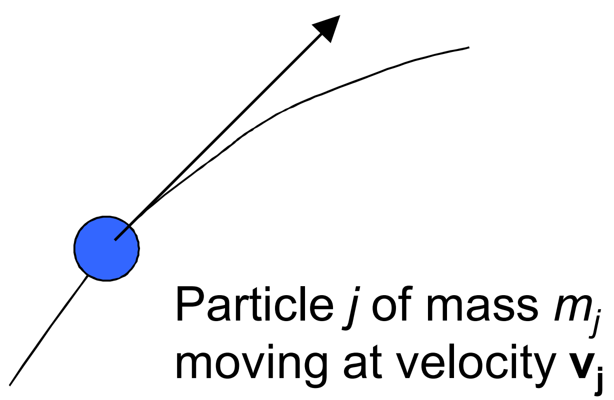
Meshless Our computation points are **particles** that now **move** according to governing dynamics , e.g. Navier-Stokes Equations

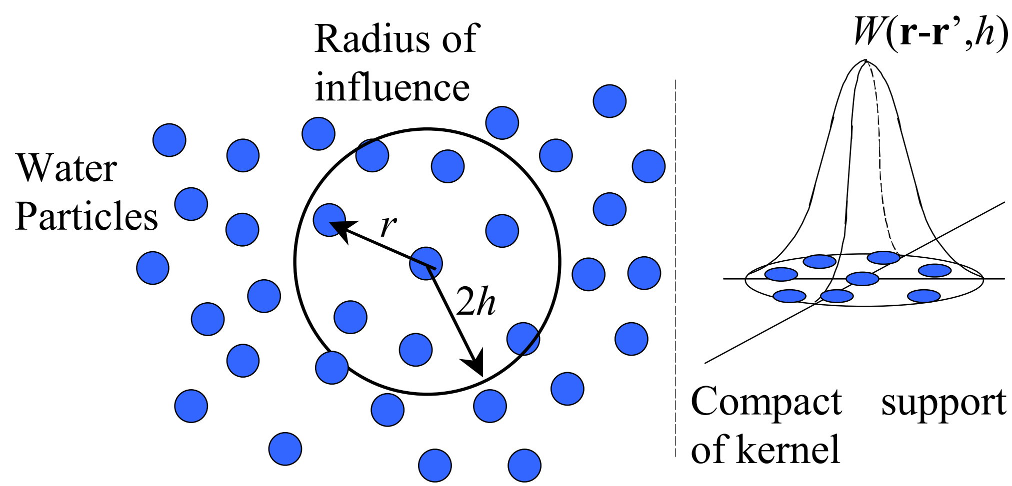
Particles move along a trajectory by **integrating** in time their velocity & acceleration

Particles possess **fluid properties** that travel with them, e.g. density, pressure; these can change with time

Local Interpolation (summation) with a **weighting function** (kernel) around each particle to obtain fluid properties

$$\langle A(\mathbf{r})\rangle \approx \sum_{j=1}^{N} A_j\, W(\mathbf{r}-\mathbf{r}_j, h)\frac{m_j}{\rho_j}$$





Equations of Motion: Approximated by Summation

- Navier-Stokes equations:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla.\mathbf{v}$$

- Are recast in

(XSPH - Mo

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{v}_i + \varepsilon\sum_j$$

$$\left(\frac{\mathrm{d}m_i}{\mathrm{d}t} = 0\right)$$

$$\mathbf{u}_j\Big) + \mathbf{F}_i$$

(I use *i* and *j* to den

Main points are that:

(i) we do not need to treat the **free surface**

(ii) No expensive meshing

(iii) SPH is Meshless & can therefore capture nonlinearity

This is the classical SPH form, we will change this!

SPH for fluid flows

What can SPH offer?

What can SPH do that other models cannot?

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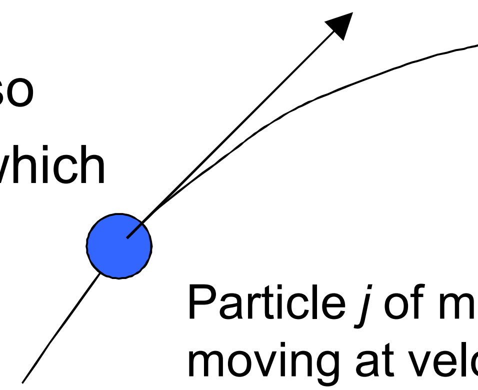
What can SPH offer the simulation of nonlinear flows?

SPH is a Lagrangian method

(a) Our computation point are the particles so we can track what happens to the particles which represent the water, the sediment, etc.



Particle *j* of mass m_j moving at velocity $\mathbf{v_j}$

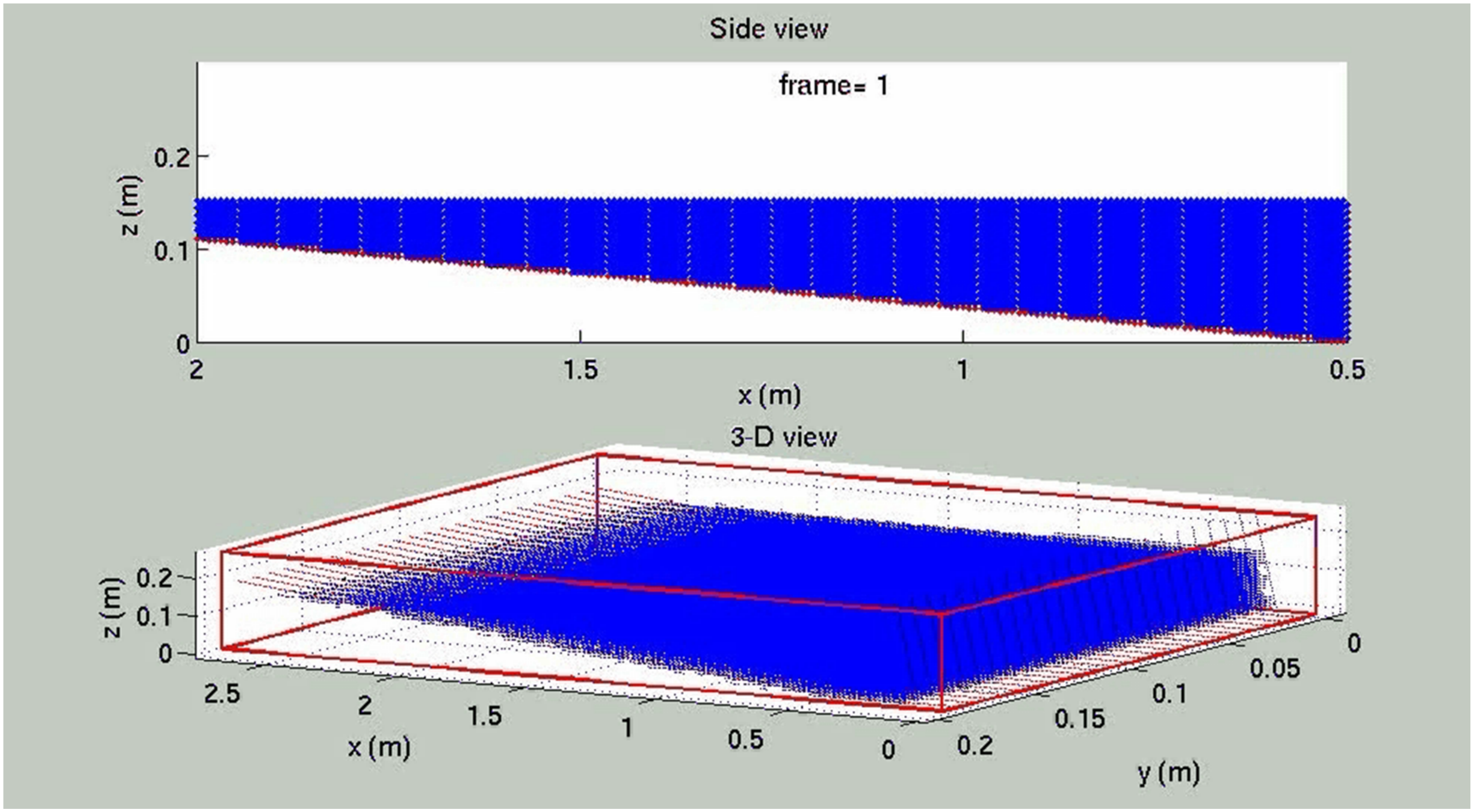
(b) This means we **avoid** the computation of the **nonlinear advection terms** within SPH

$$\frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla \Rightarrow \frac{D}{Dt}$$

Only the RHS of our equations need SPH treatment

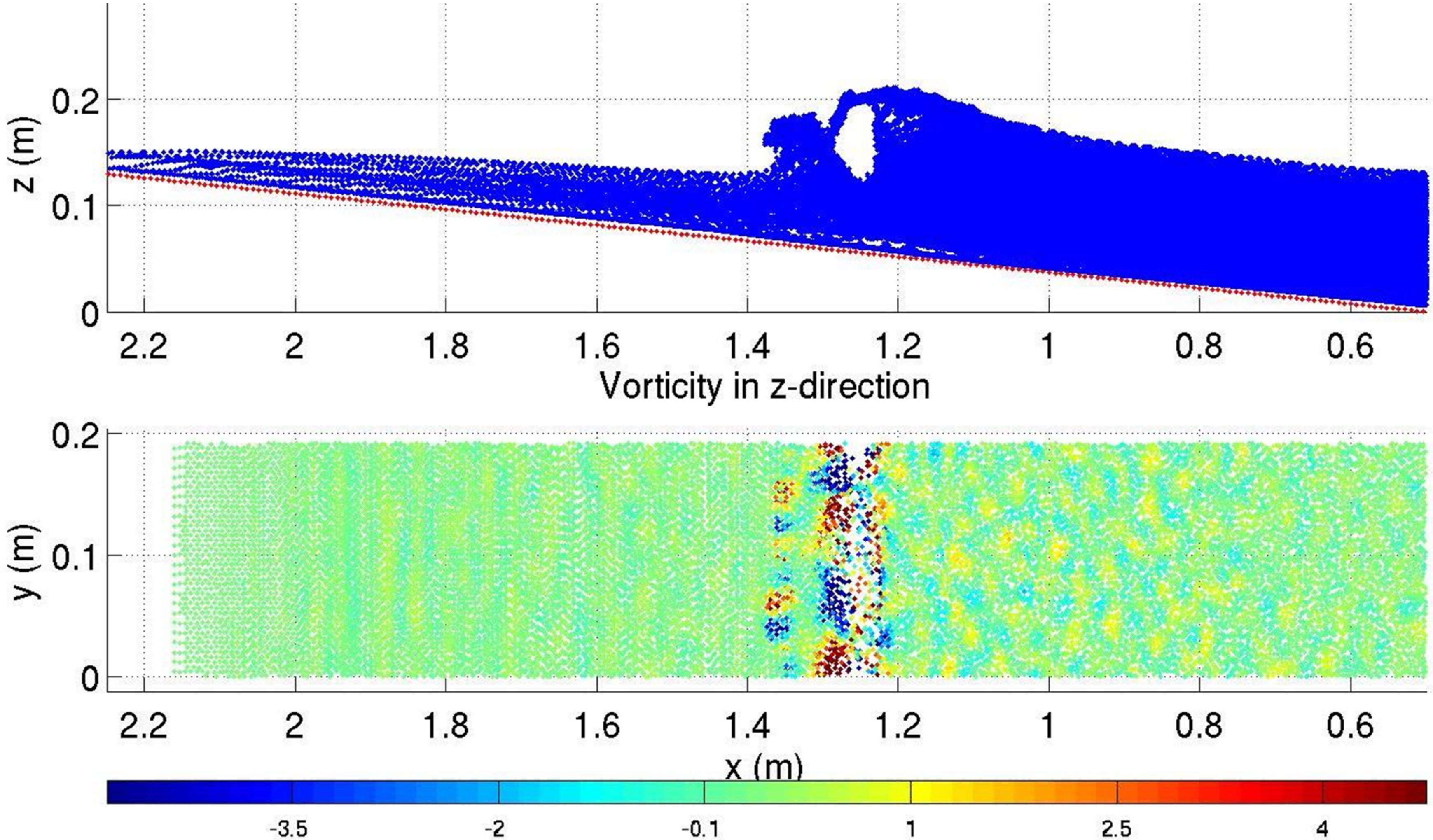
This makes nonlinear phenomena very easy to examine, in particular **FORMATION mechanisms**, eg. mixing …

WAVES 2005: Captured Obliquely-Descending Eddies (ODEs) in 3-D



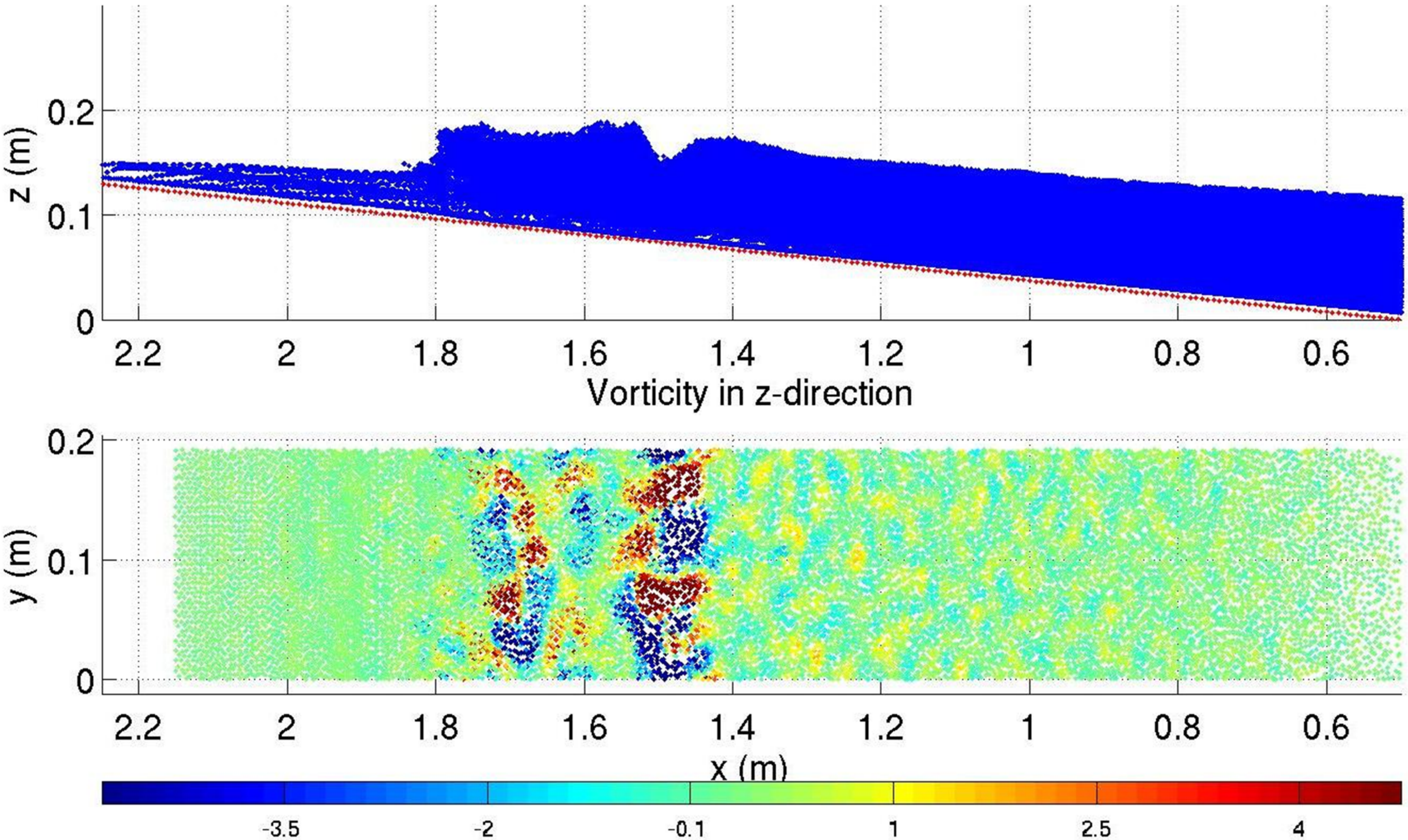
- Rogers & Dalrymple (2005)

WAVES 2005: Captured Obliquely-Descending Eddies (ODEs) in 3-D

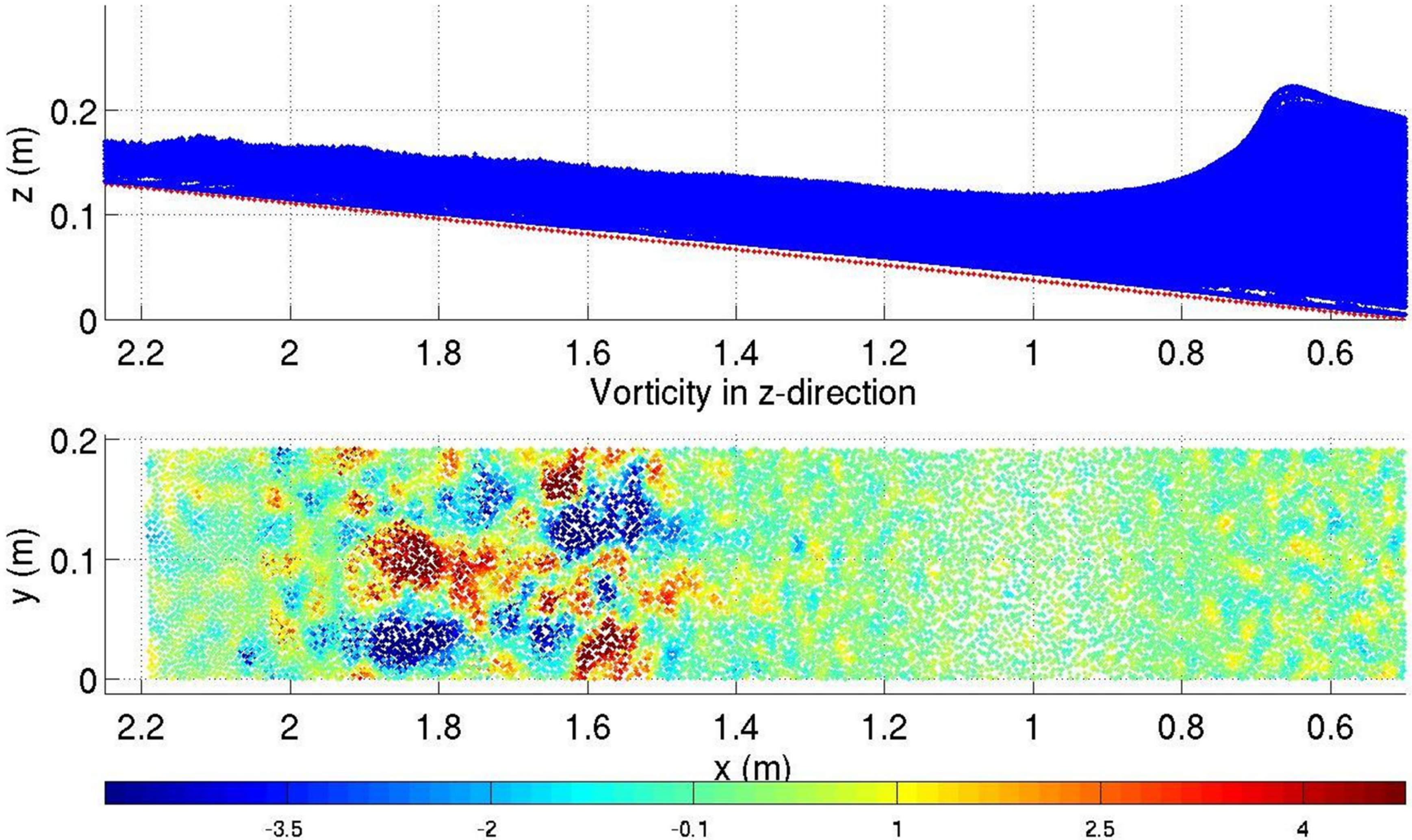


Initiating turbulence

WAVES 2005: Captured Obliquely-Descending Eddies (ODEs) in 3-D



WAVES 2005: Captured Obliquely-Descending Eddies (ODEs) in 3-D



DualSPHysics - what is it?

Where did DualSPHysics come from?

What can DualSPHysics offer?

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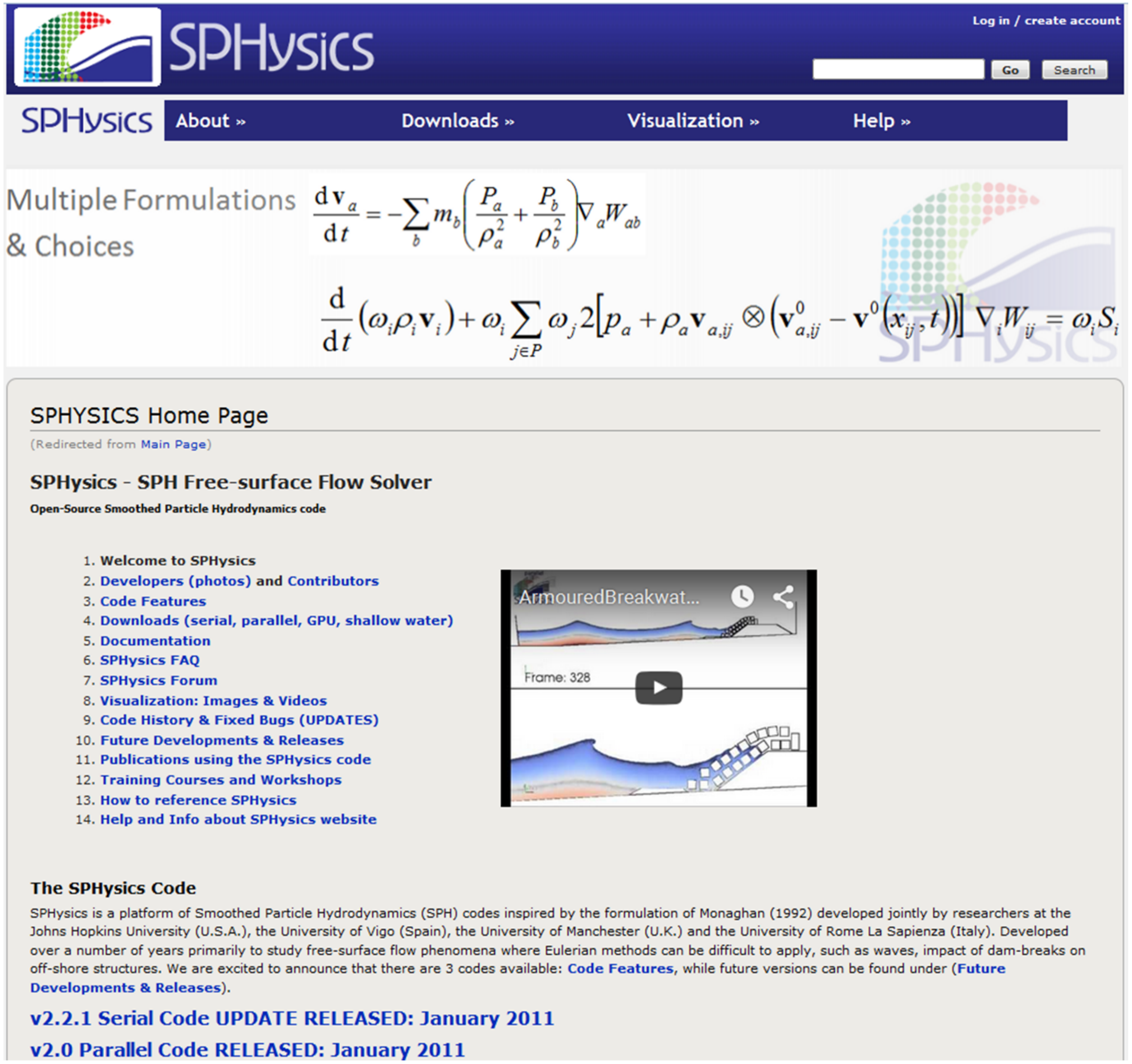
DualSPHysics History - SPHysics

FORTRAN → **CUDA/C++**

SPHysics – 1st open-source code for free-surface flow (FORTRAN)



Result of 8 years of work

Released in 2007

Collaboration between 4 institutions

- University of Manchester
- Universidade de Vigo
- Johns Hopkins University
- University of Rome La Sapienze

SPHysics – 1st open-source code for free-surface flow (FORTRAN)

- Code had 5 test cases
- 2-D & 3-D
- Choice of options beyond anything else available: kernels, timestepping, formulations & completely open source (mistakes, coding tricks, …)
- Importantly it was VALIDATED against simple cases

BUT

- It was very slow
- Restricted to 250,000 particles (simulations took 2-3 weeks)
- Had primitive pre- and post-processing

DualSPHysics History - GPUs

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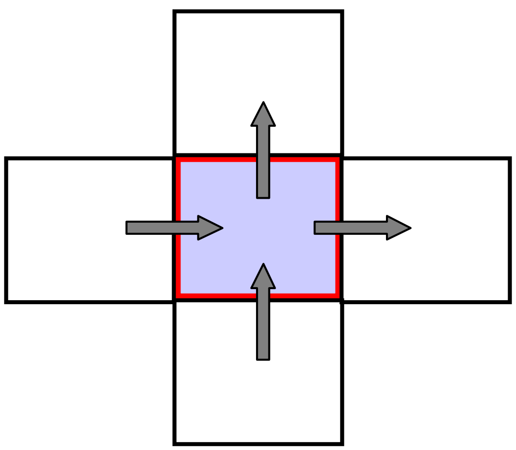
SPH ***was*** prohibitively expensive computationally

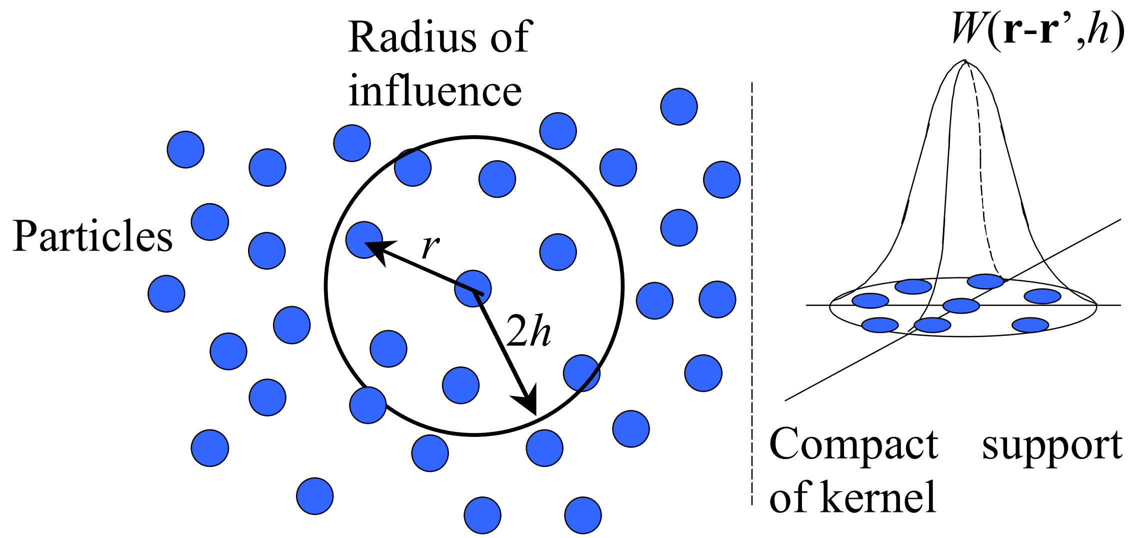
SPH is costly computationally, Why?

- The main problem is due to the interpolation procedure itself
- In Finite Volume, Finite Element & Finite Difference Schemes, the stencil around any cell usually contains only a small number of neighbouring cellsl e.g. **In 2-D FVM only 4 neighbouring cells**

Finite Volume (FVM) Stencil



SPH Stencil



- In **2-D**, each particle typically interacts with **20-50 particles**
- In **3-D**, each particle typically interacts with **100-400 particles**

Hardware Acceleration: the options

(i) Using parallel (**supercomputer**) machines with lots of cores (individual CPUs) and divide the work over them

Qu: What's the difference between a parallel machine and a supercomputer?

(ii) **FPGAs** – Field Programmable Gate Arrays: well used in astrophysics simulations, but expensive and not portable

(iii) **GPUs** – Graphics Processing Units: the **hot topic** of scientific computing

TOP SUPERCOMPUTERS IN THE WORLD Nov 2016

http://www.top500.org

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

TOP 10 Sites for November 2016

1º	Sunway Taihulight (China)	93.0 petaflops/s	(consumption: 15371 KW)	(CPUs)
3º	Titan (USA)	17.5 petaflops/s	(**consumption: 8209 KW**)	(**with GPUs**)

Rank Site System Cores (TFlop/s) (TFlop/s) (kW)

Energy Efficient GPU co-processors are now a key component in HPC

Part of computing Emerging Technology 2016 Conference:

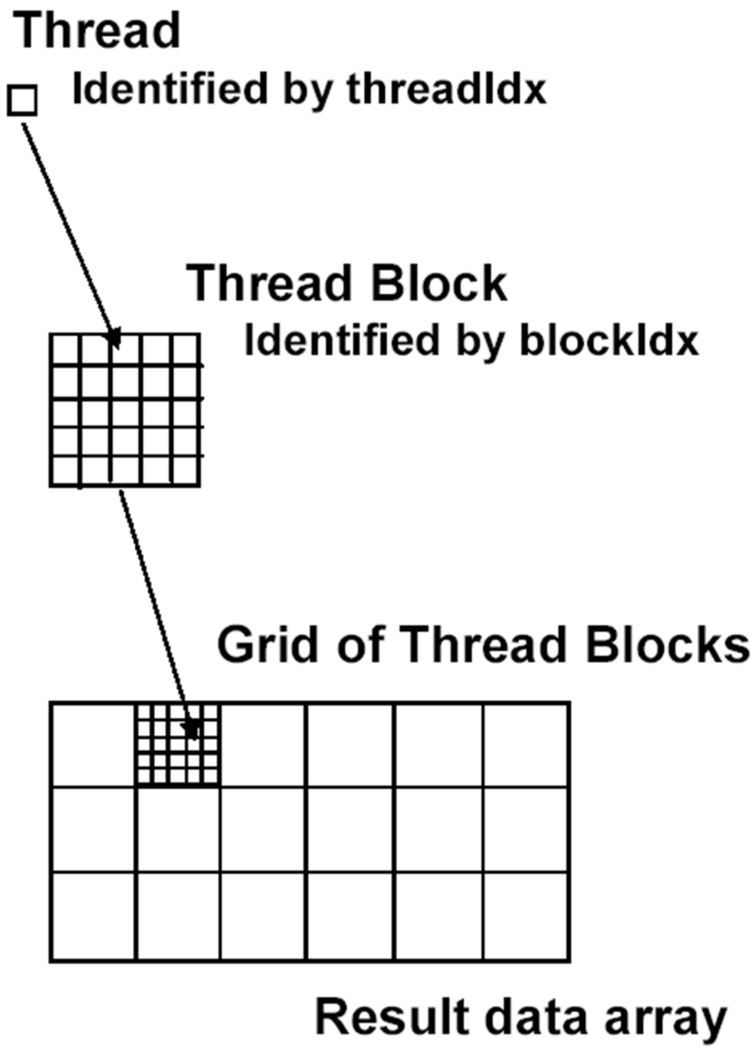
http://emit.tech

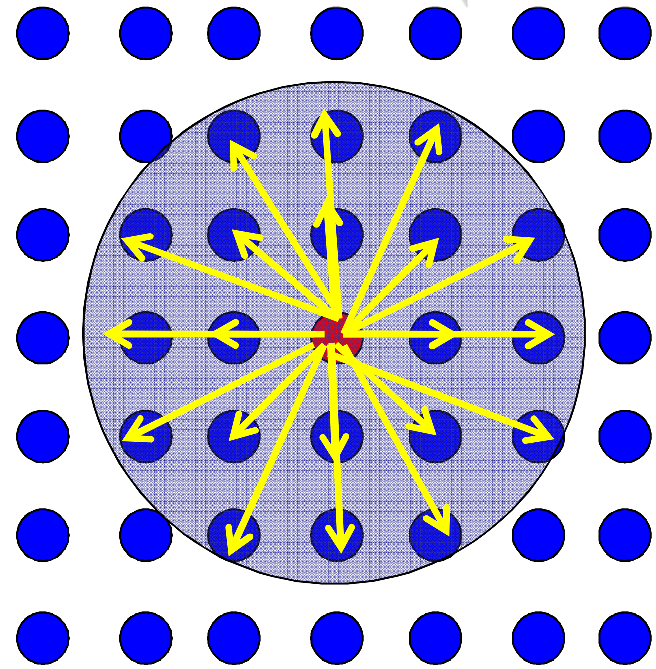
High Performance Computing Japan — M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path Fujitsu

There are now several GPU codes …

SUMMATION SOLUTION

GPU / CUDA

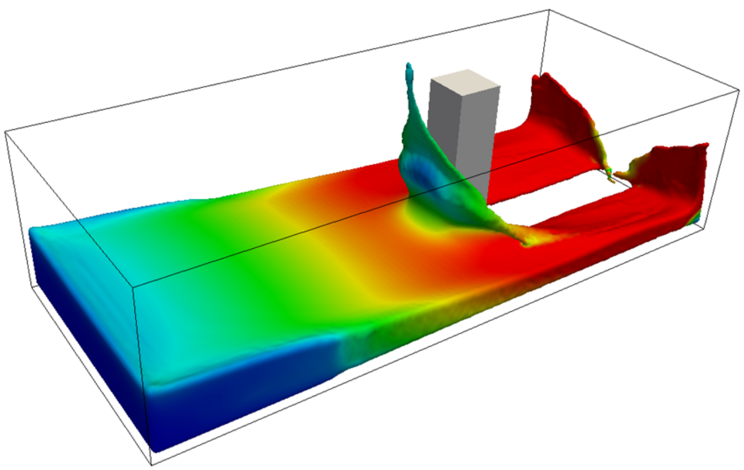


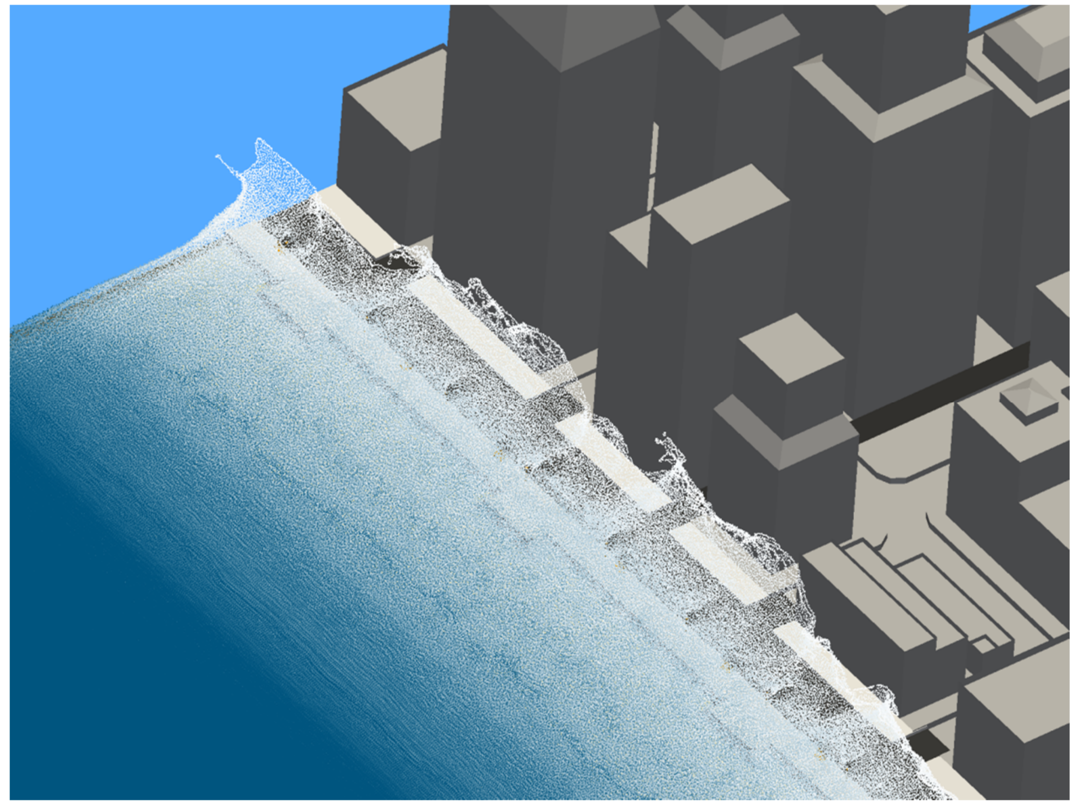


$$\left(\frac{d\mathbf{u}}{dt}\right)_i = -\sum_j m_j\left(\frac{p_j}{\rho_j^2}+\frac{p_i}{\rho_i^2}\right)\nabla_i W_{ij} + \mathbf{g}$$

$i \rightarrow j$

DualSPHysics, new GPU computing on SPH models





A.J.C. Crespo, J.M. Dominguez, A. Barreiro and M. Gómez-Gesteira
EPHYSLAB, Universidade de Vigo, SPAIN

B. D. Rogers and D. Valdez-Balderas
MACE, The University of Manchester, U.K.

Universidade Vigo

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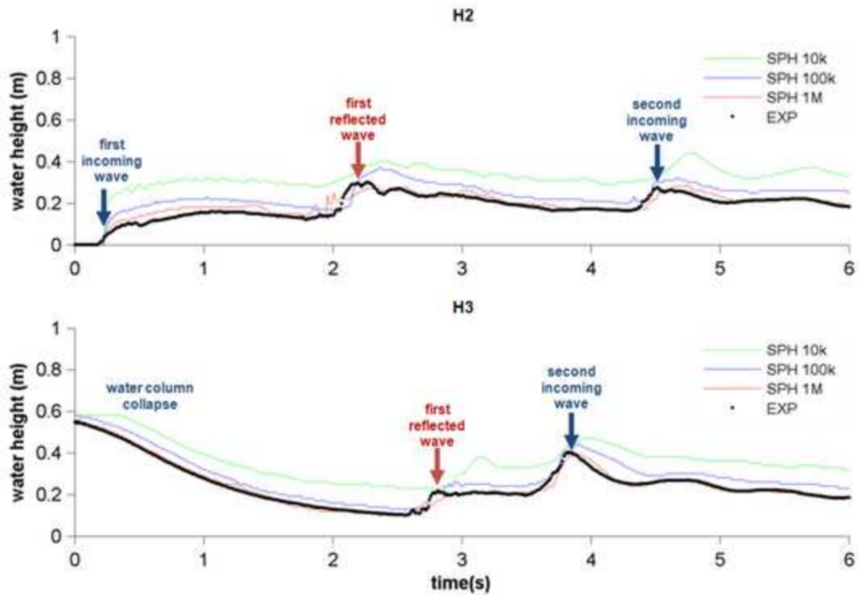
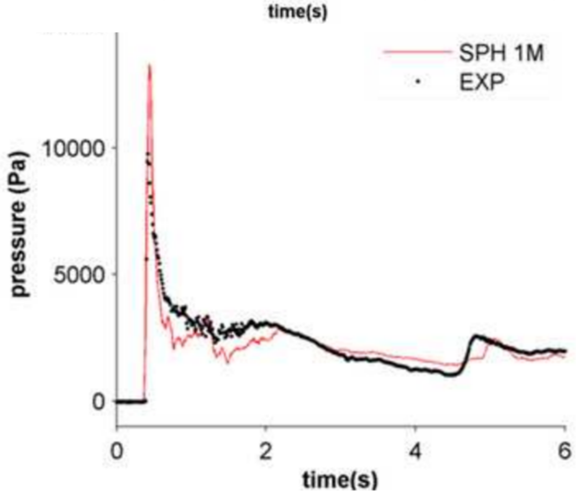
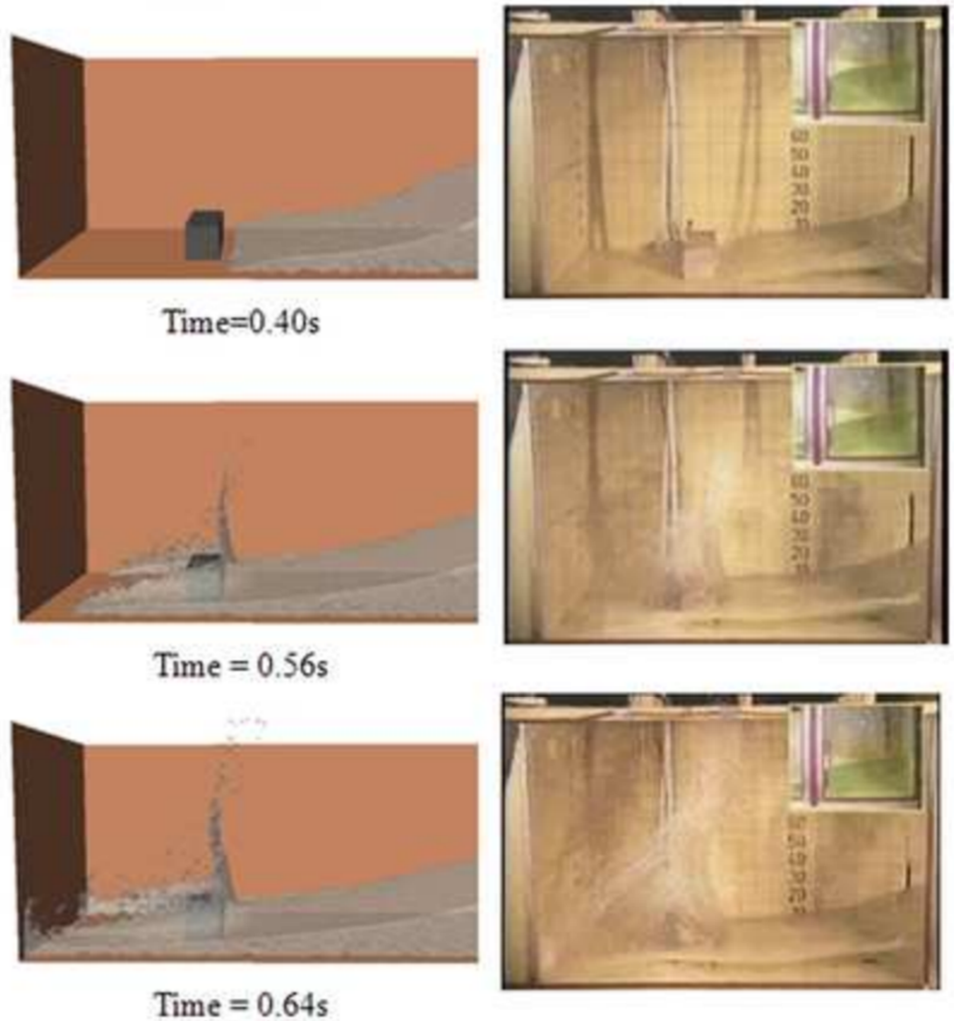
GPU validation for a dam break flow impacting on an obstacle

SPHERIC BENCHMARK TEST CASE 2

Crespo AJC, Dominguez JM, Barreiro A, Gómez-Gesteira M and Rogers BD. 2011. *GPUs, a new tool of acceleration in CFD: Efficiency and reliability on Smoothed Particle Hydrodynamics methods.* PLoS ONE. doi:10.1371/journal.pone.0020685





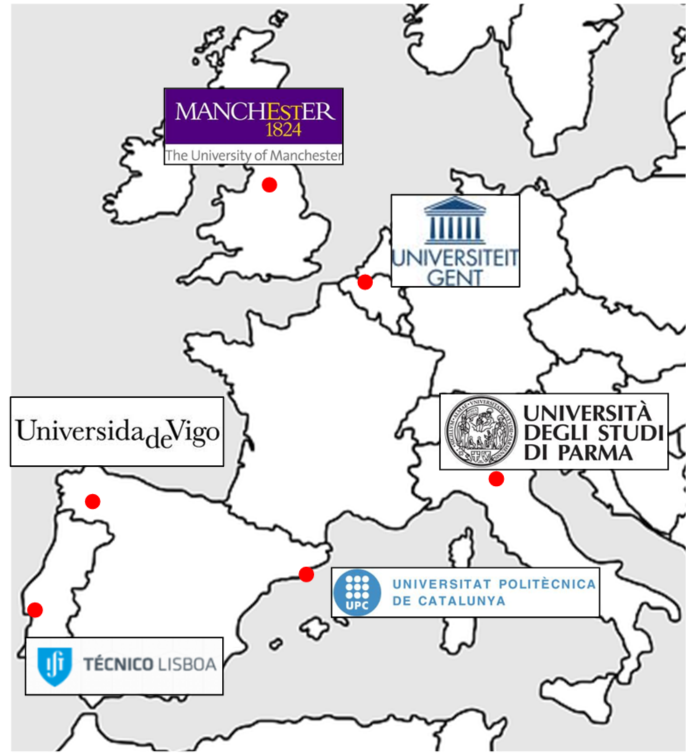


The DualSPHysics project team

Who are we?

DualSPHysics Project:

- University of Manchester
- University of Vigo (Spain)
- University of Parma (Italy)
- University of Lisbon (Portugal)
- University of Ghent (Belgium)



Websites

- Free open-source **SPHysics** code:

  http://www.sphysics.org

  http://www.dual.sphysics.org

Downloaded 15,000+ times: The world's 1st open-source plug & play SPH code for free-surface flow

The DualSPHysics Areas of Activity

What do we do?

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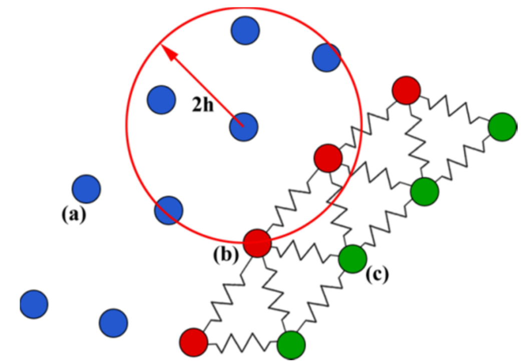
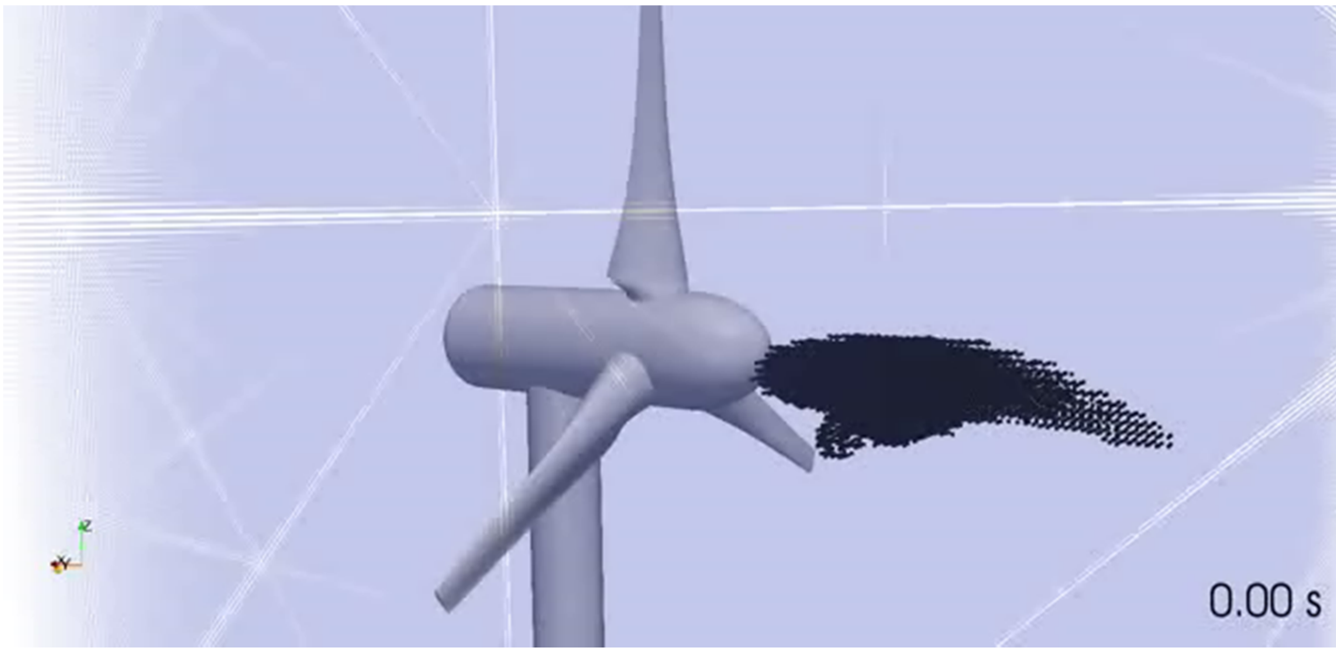
Combined SPH-MSD Simulation

After many validation cases:





Involves different Young's moduli of elasticity for different elements of whale

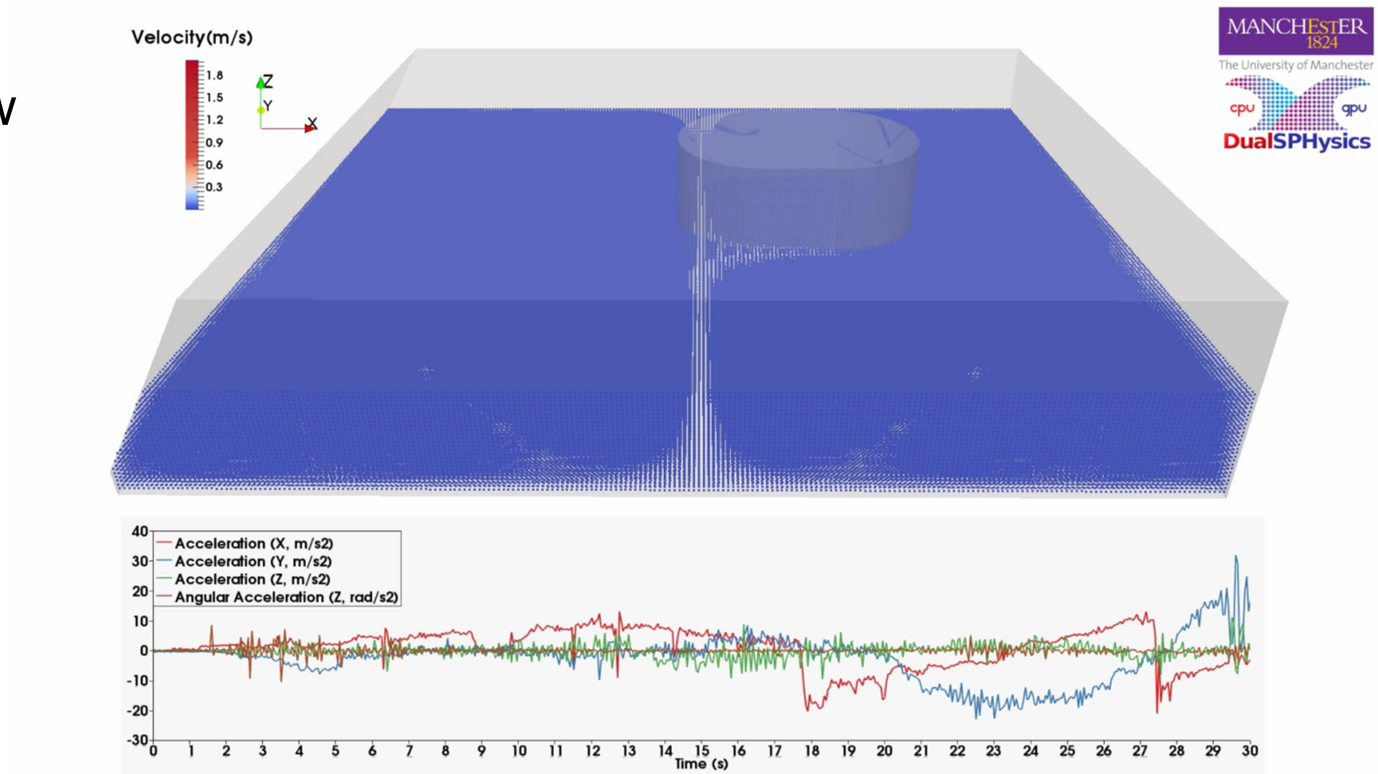
Fuel-tank sloshing with Leading Motorsport Company (F1)

Real engineering problems are now accessible

Only allowed to show highly simplified geometry

Accelerations are up to 5*g*

Comparisons with in-tank footage were close.



Longshaw & Rogers (2015), Advances Engineering Software

Funded by Knowledge Transfer Account (KTA), *now the IAA*

Manchester SPH Activity

What work do we do at Manchester?

Better SPH: The options

1. ~~Density filtering~~

$$\rho_a^{new} = \sum_b \rho_b \widetilde{W}_{ab} \frac{m_b}{\rho_b} = \sum_b m_b W_{ab} \Bigg/ \sum_b W_{ab} \frac{m_b}{\rho_b}$$

Dissipative

2. Volume diffusion methods:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_j m_j \left(\mathbf{v}_i - \mathbf{v}_j\right) \nabla_i W_{ij}$$

$$\Rightarrow$$

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_j m_j \left(\mathbf{u}_i - \mathbf{u}_j\right) \nabla_i W_{ij} - \frac{\mathbf{r}_{ij}}{r_{ij}} \cdot \nabla_i W_{ij} \left(\frac{c_{ij}}{\rho_j} \left(\rho_j - \rho_i\right) \right)$$

3. Introducing ALE formulations & Riemann solvers

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij}$$

$$\Rightarrow$$

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_j m_j 2P_{ij}^* \left(\frac{1}{\rho_i^2} + \frac{1}{\rho_j^2} \right) \nabla_i W_{ij}$$

4. Incompressible SPH (ISPH) **+ shifting (unique Manchester project)**

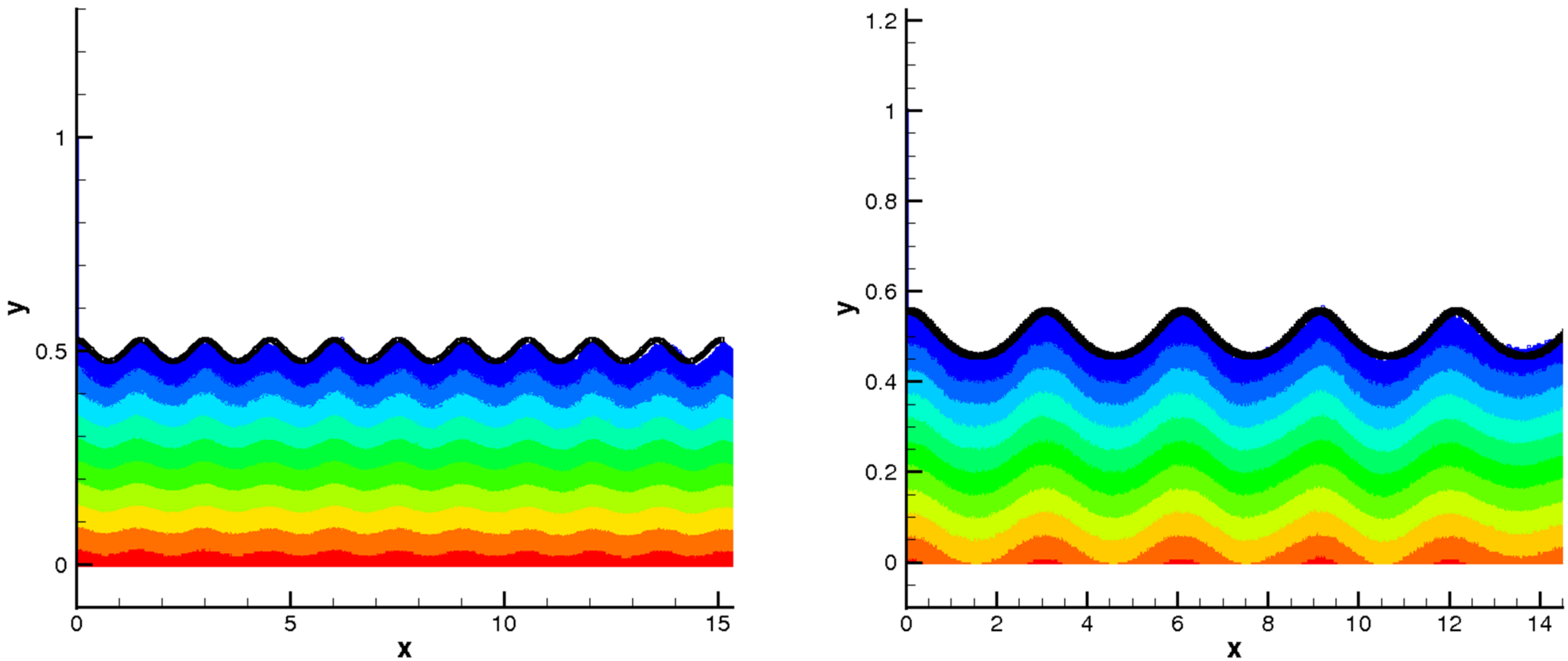
$$\nabla \cdot \left(\frac{1}{\rho} \nabla p^{n+1} \right)_i = \frac{1}{\delta t} \nabla \cdot \mathbf{u}_i^*$$

$$\Rightarrow$$

$$\delta \mathbf{r}_s = -\mathcal{D} \left(\frac{\partial C}{\partial s} \mathbf{s} + \alpha \left(\frac{\partial C}{\partial n} - \beta \right) \mathbf{n} \right)$$

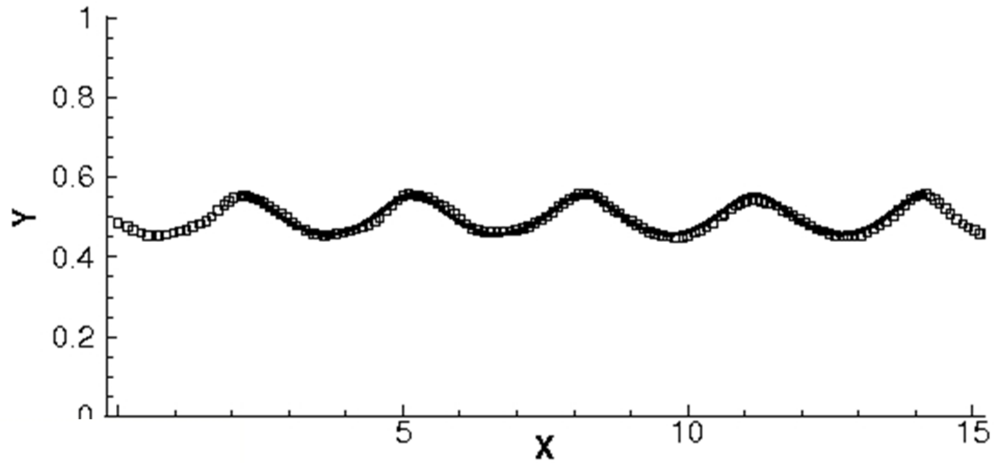
Shift particles to maintain stability.

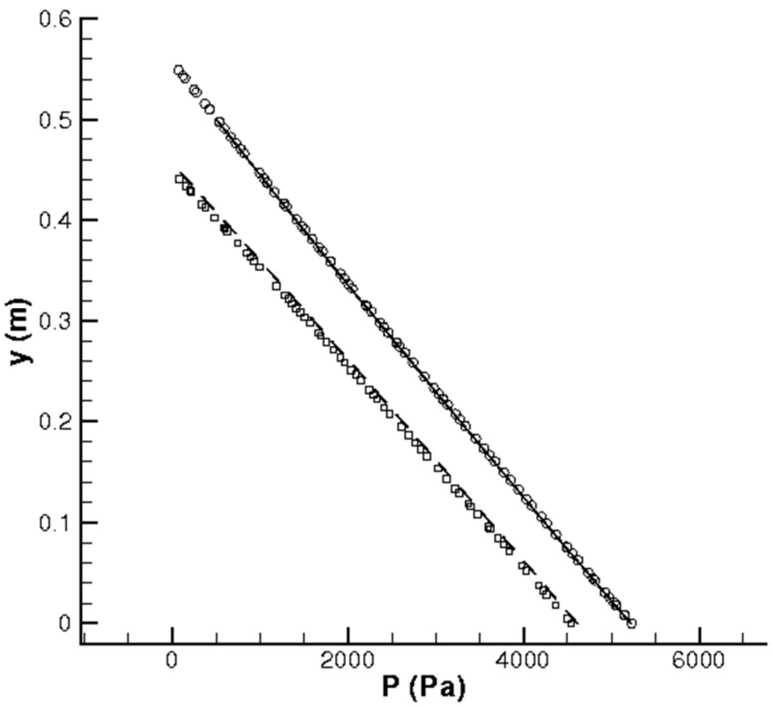
Improvement in wave propagation using Incompressible SPH

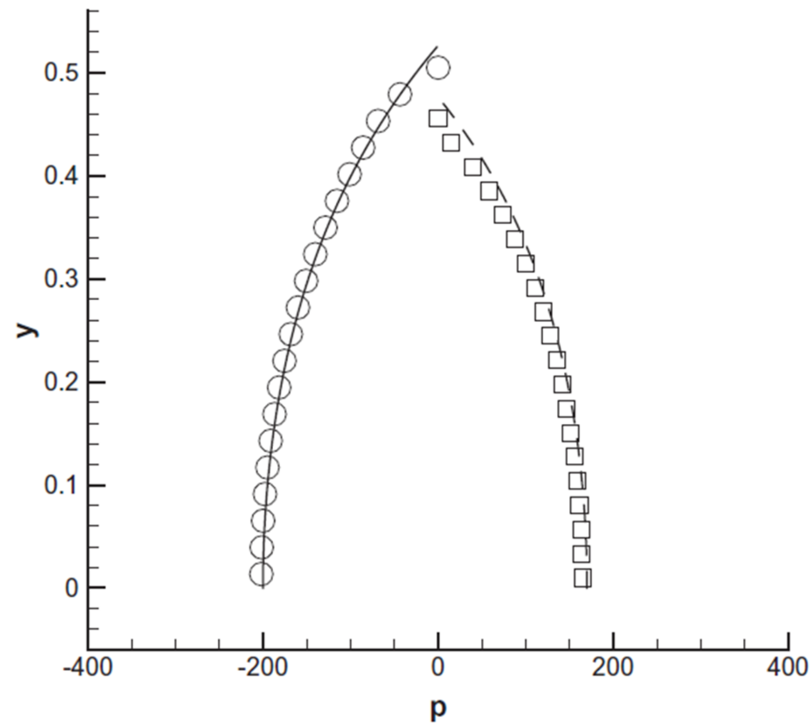


Comparison of wave propagation along a channel (including pressure contours) with free-surface predictions of SAWW (bold black line).
(a) Wave height *H = 0.05m at t = 19.5s. (b) Wave height H = 0.1m at t = 9.75s.*

Free surface in the regular wave case. Square symbols = ISPH; solid line = code SAWW Squares = ISPH; solid lines = code SAWW. Time = 12.53s, wave height H = 0.1m, wave length = 3.0m.







Full & Dynamic Pressure along the vertical line at cross sections, wave crest & trough. Solid lines = wave crest, code SAWW; dashed lines = wave crest, code SAWW; circles = wave crest, ISPH; diamonds = wave crest, ISPH.

Eulerian SPH

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Mixed Eulerian-Lagrangian ISPH

Increased accuracy and efficiency

Fourtakas *et al*. (2016)

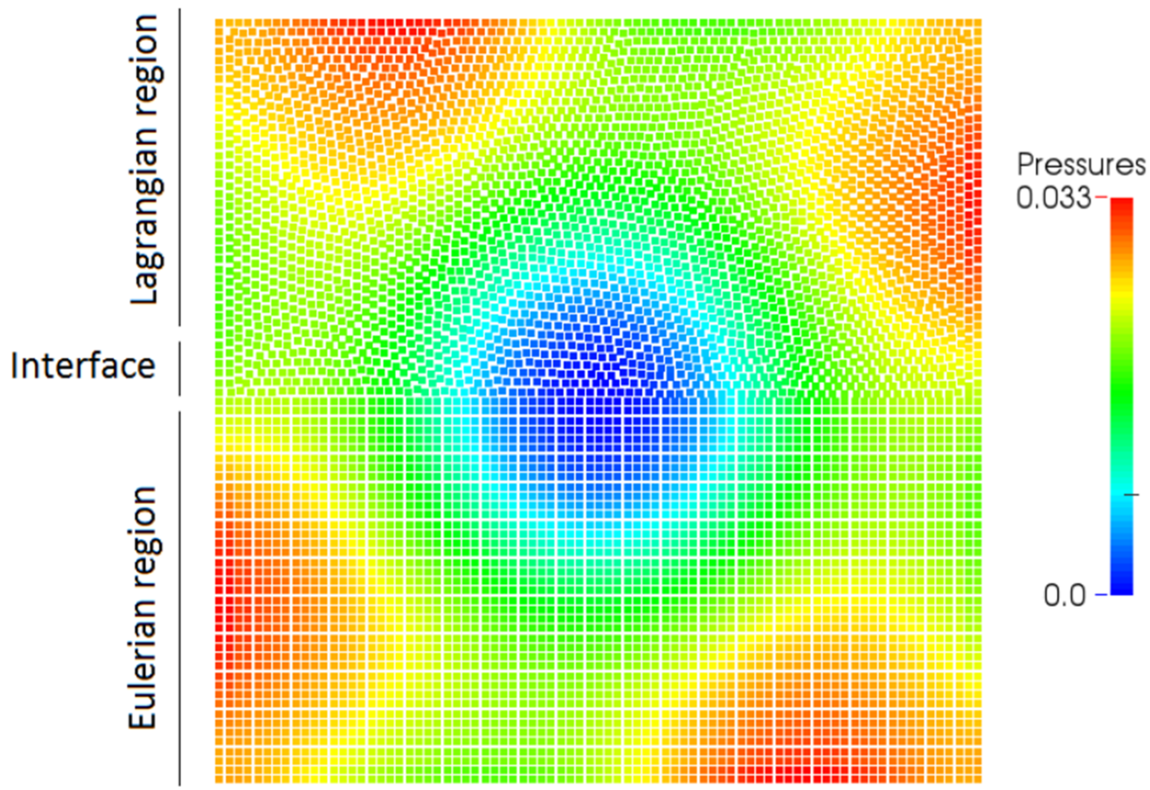
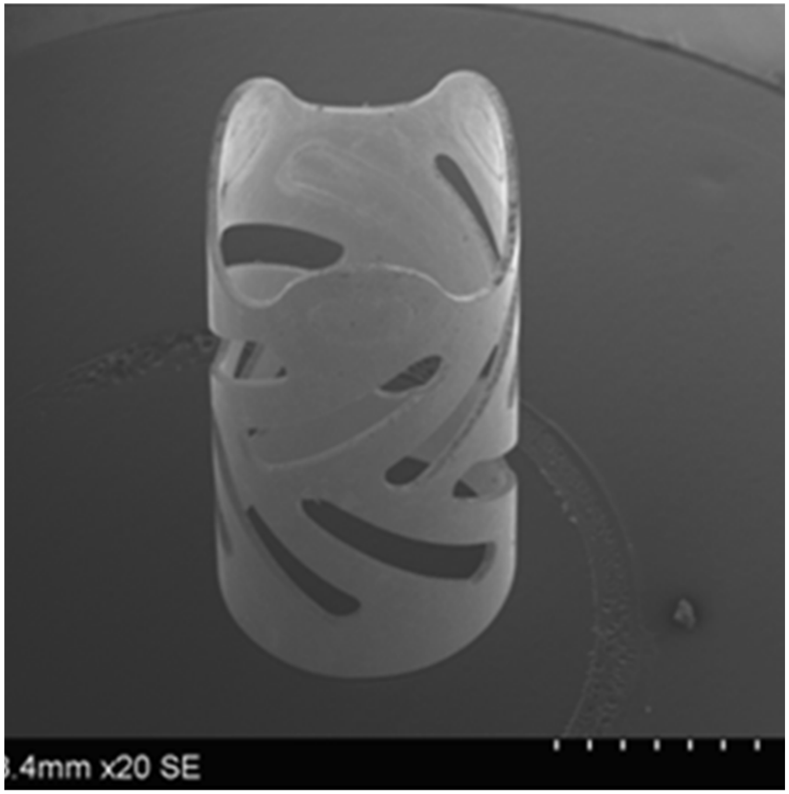


Figure 12. Horizontal and verical velocity profiles of the vortex spin-down case for dx = 0.0125 with *Re* = 1000 *t* = 10 s.

Now ***multi-phase ….***

Laser Cutting Applications

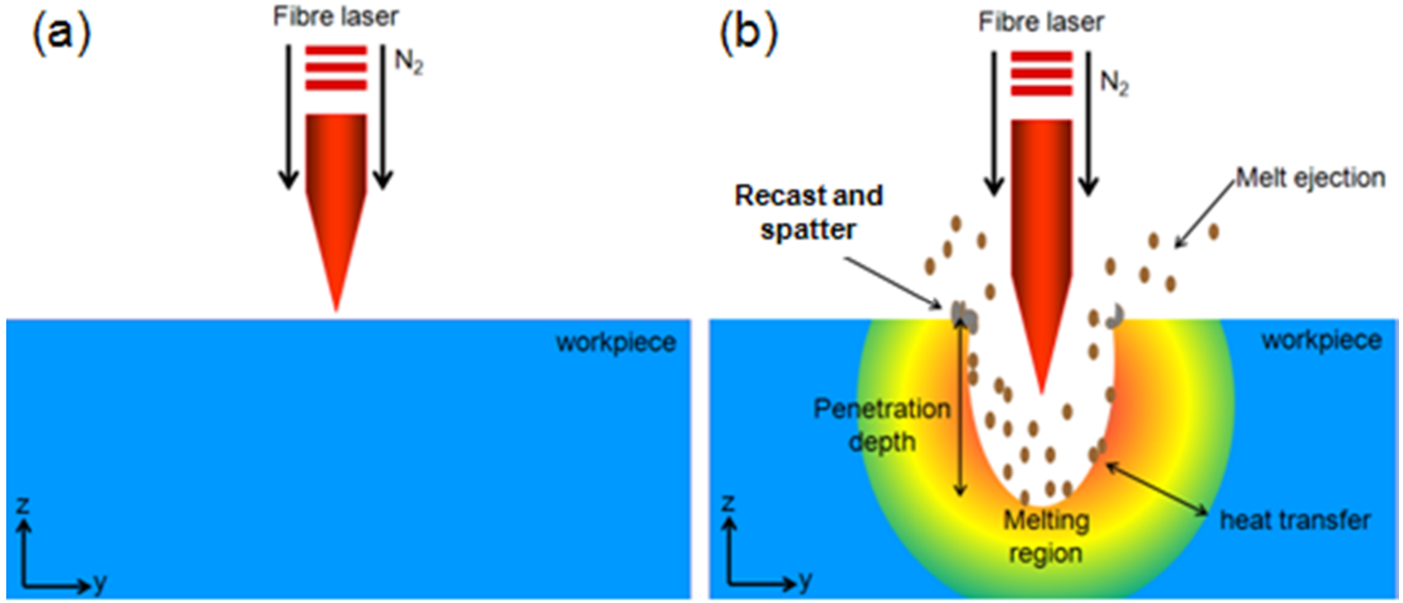


platinum

SEM images of laser cut samples:

- Laser beam heats the surface of the object in **very short pulses** (typically ms to ps)
- For ms heating, the surface particles increase in Temperature, melt & leave the surface – ideal for SPH
- Backwall damage and debris result
- Assist gas helps the removal of particles within the cut
- Water removes particles under the cut

Laser Cutting Process 1



Heat Transfer

$$c_p \frac{dT}{dt} = \frac{1}{\rho}\nabla(k\nabla T) + Q - Q_v$$

SPH

$$c_{p,i}\frac{dT_i}{dt} = \sum_j \frac{m_j}{\rho_i \rho_j}(k_i + k_j)\left(\frac{T_i - T_j}{\mathbf{r}_{ij}^2}\right)\mathbf{r}_{ij}.\nabla_i W_{ij} + Q - (Q_v)$$

Laser Beam

$\rho_m = \rho(T)$

Laser changes Temperature & density

⇨

$$P_{vap} = P_0 \exp\left[\frac{L_v}{R}\left(\frac{1}{T_b} - \frac{1}{T_s}\right)\right]$$

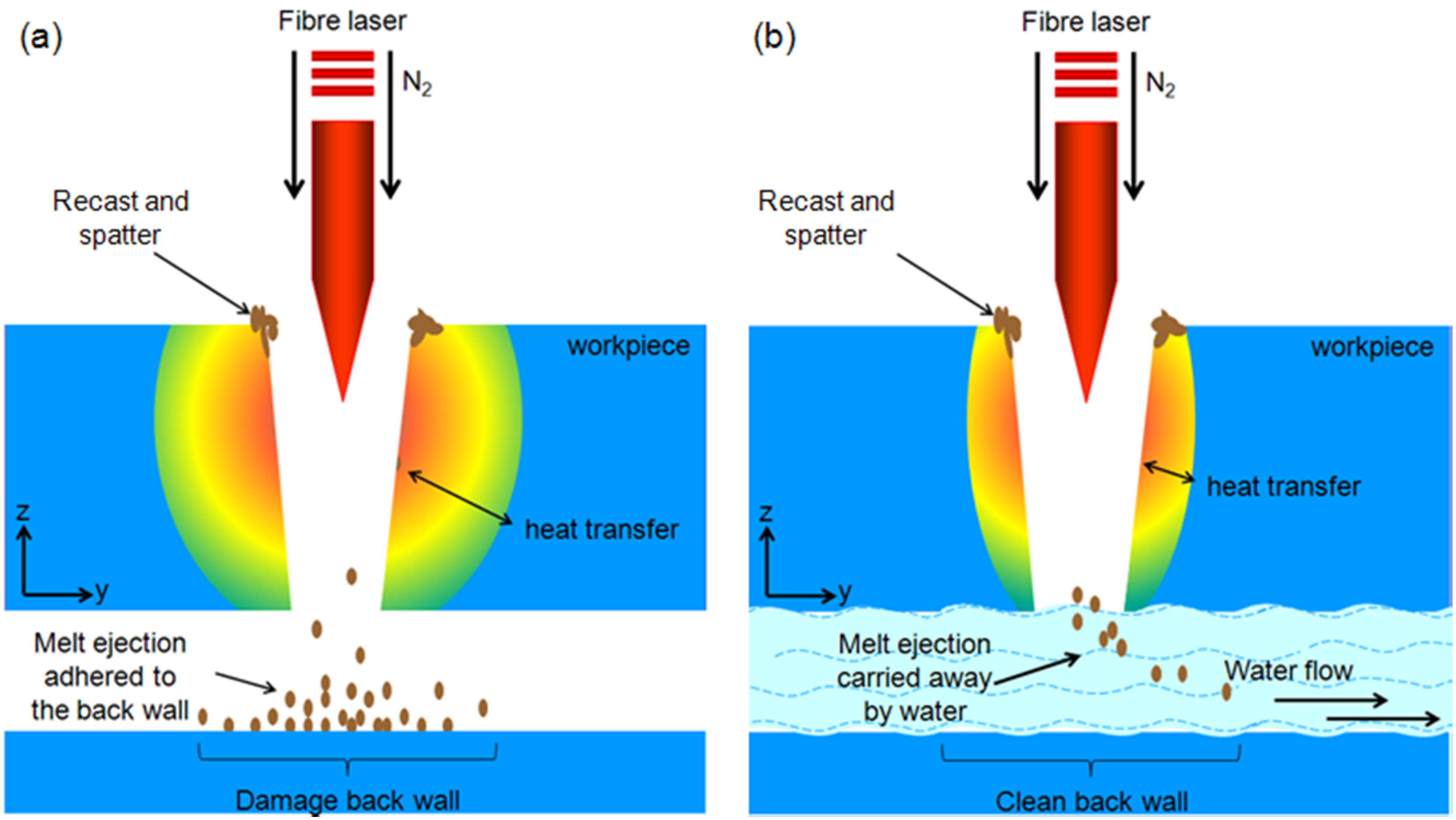
Changes in surface temperature & pressure

⇨

$$V_m = \sqrt{\frac{2(P_{vap} + P_{eff})}{\rho_m}}$$

Ejection velocity with assist gas N_2

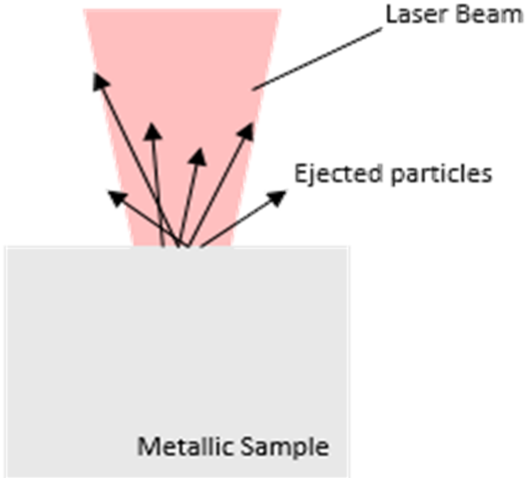
Dry & Wet Laser Cutting

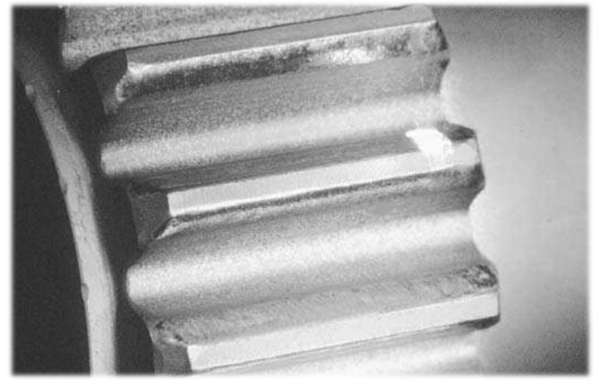


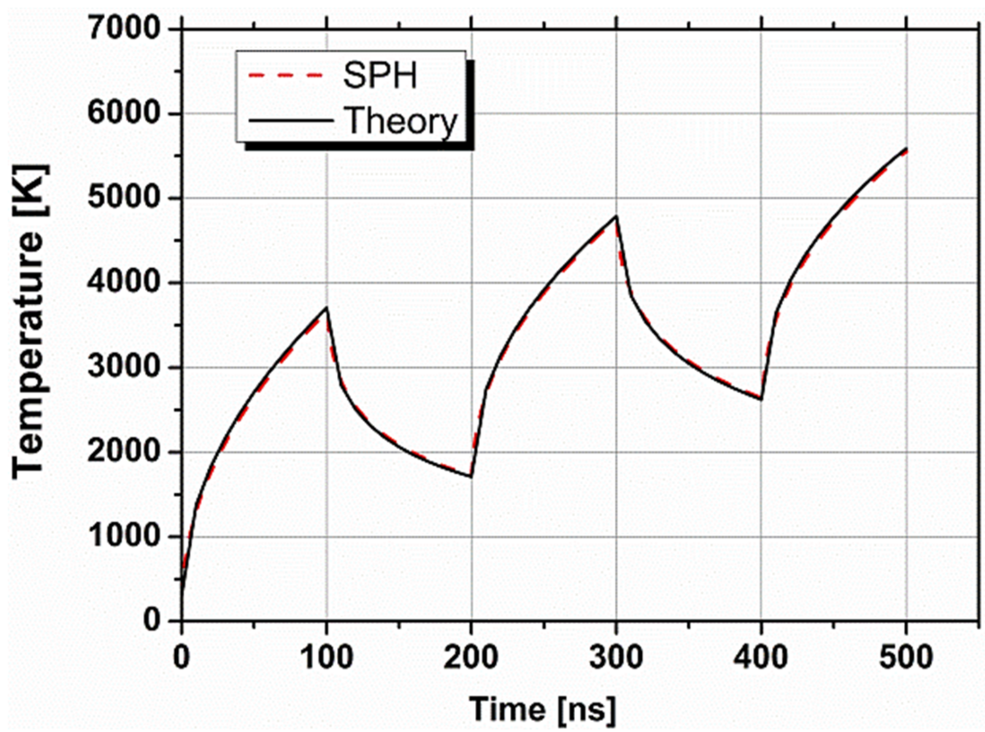
In both cases, the solid phase changes directly into the gaseous phase

We are not modelling Molecular Dynamics, but use continuum description & SPH to represent the physics.

Laser Ablation







ns and ps pulses generated large increases in Temperature

(Al-Shaer *et al*. 2016 *Computational Materials Science*)

Psyllaki, P., and Oltra, R., 2000, Materials Science and Engineering: A, 282(1–2), pp. 145-152

ION, J. C. (2005). *Laser processing of engineering materials principles, procedure and industrial application*. Oxford, Boston.

SPH free-surface Applications

Application: Large-scale Flooding

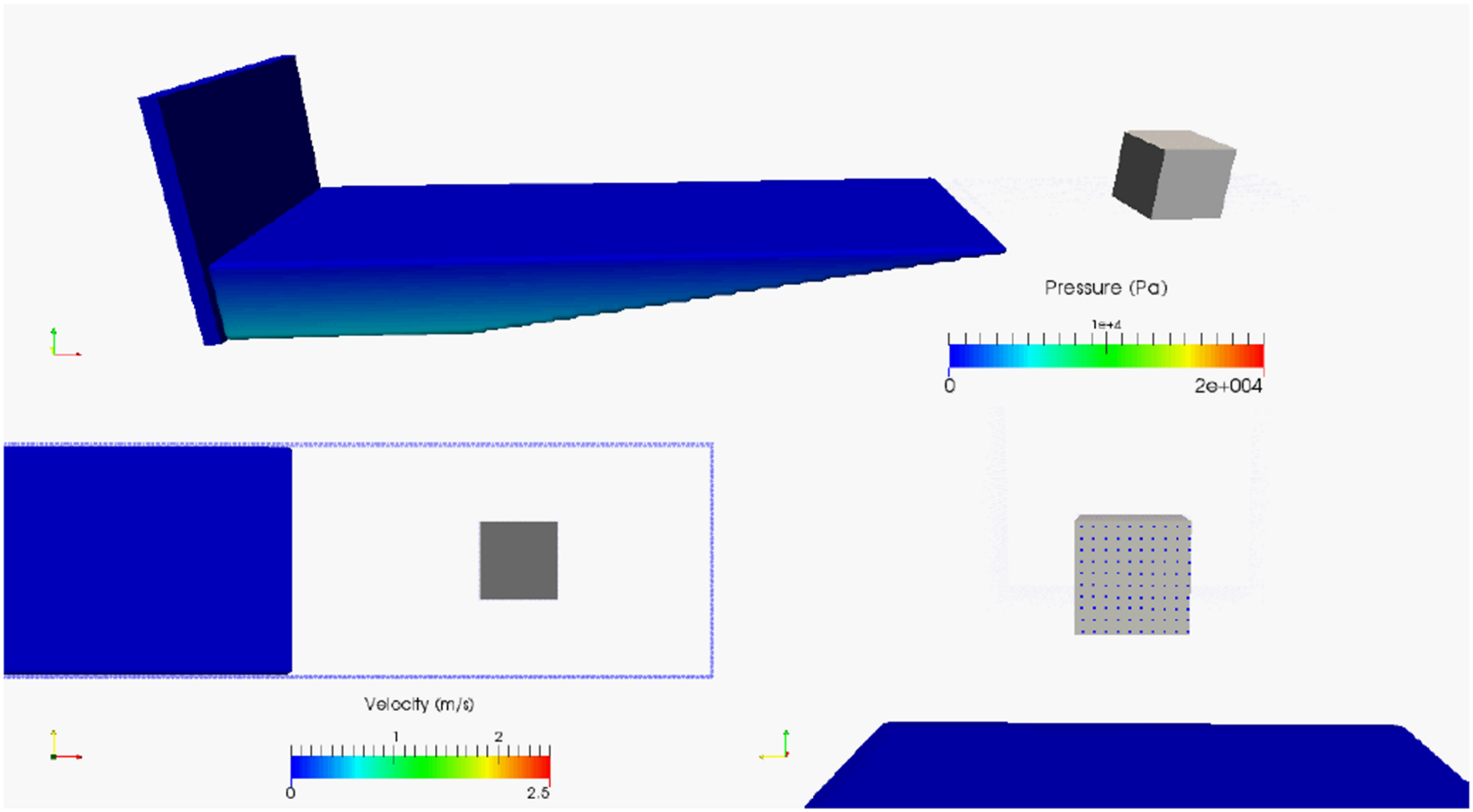
Pringgana et al. 2016, Cunningham et al. 2015

(*Proc. ICE: Engineering and Computational Mechanics*)

Tsunami-structure interaction modelling with SPH

DualSPHysics model simulation:

Side view

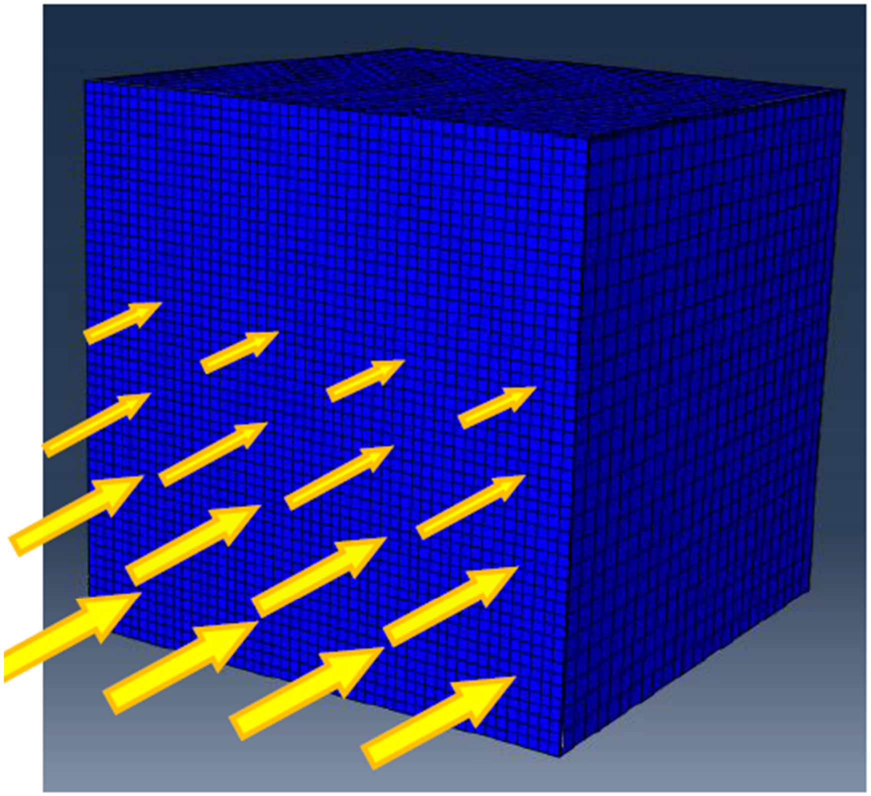


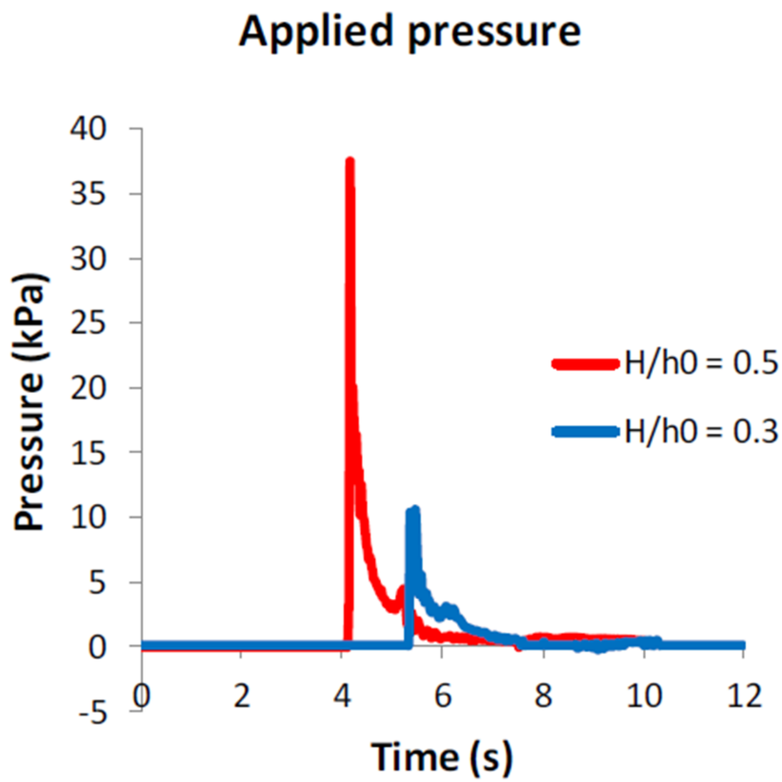
Top view

Front view

Tsunami-structure interaction modelling with SPH

FE model mesh size and applied loads





Example of load (pressure) time histories at lowest level

Tsunami-structure interaction modelling with SPH

Stress on structure's components

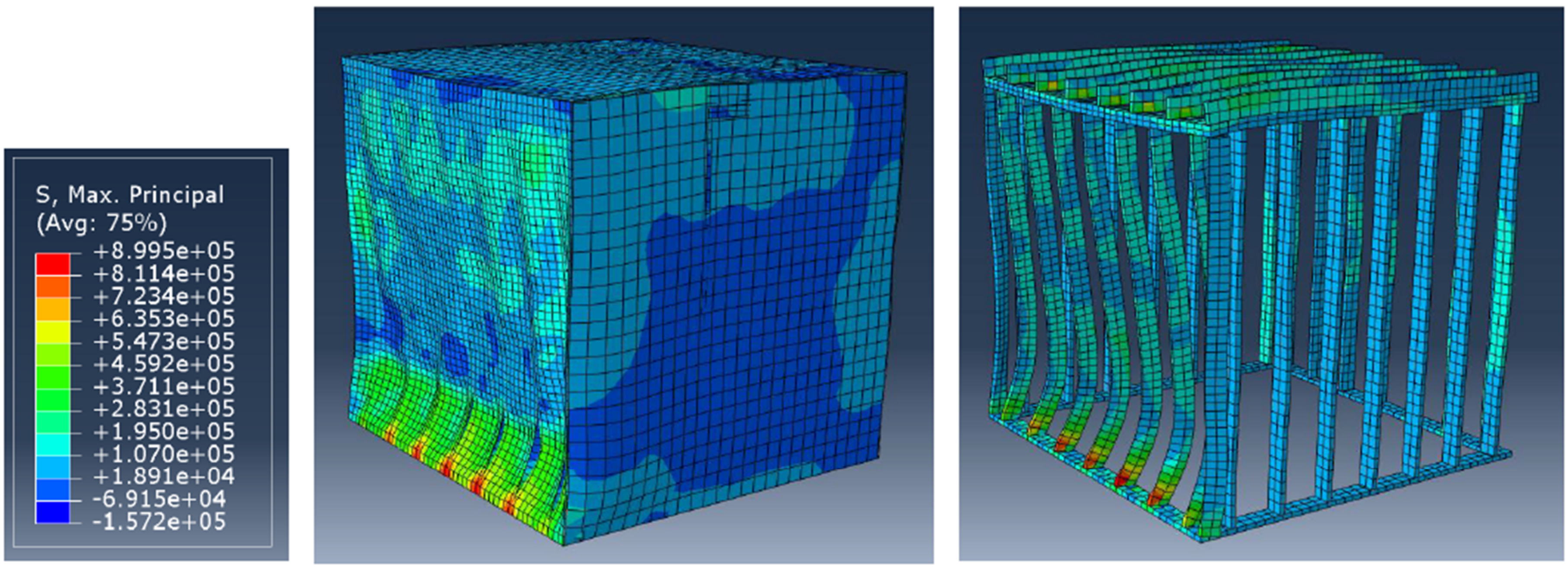
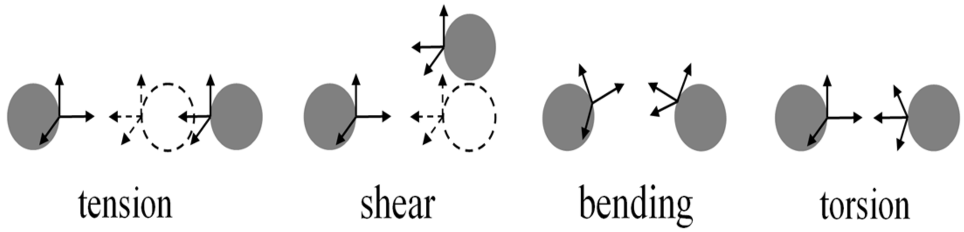


Figure: Stress (Pa) on plywood and studs at the point of maximum impact pressure

Pringgana *et al*. (2016), Cunningham *et al*. (2015), *Engineering and Computational Mechanics*. Awarded Thomas Telford Award by Institution of Civil Engineers

Vector-based Discrete Element Method (V-Model) for granular structures



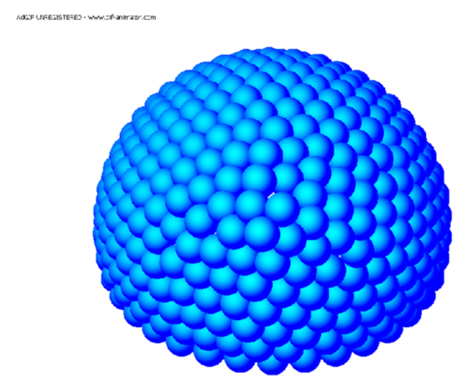
Two particle V-DEM model illustrating relative vector orientation under different deformation.

Original stiffnesses for tension, shear & bending

$$C_a = \frac{EA}{L}, C_S = \frac{GA}{L}, C_b = \frac{EI}{L}$$

V-Model (Kuzkin & Asonov 2012)

- Vectors on surface of particles define particle orientation relative to connected neighbours.
- Potential energies of bonds are a function of deformations calculated using particle surface vectors.
- Explicit method, time integration similar to SPH.
- Interactions are local making it ideal for computational parallelisation and coupling with SPH.



Buckling with point force applied at top of elastic hemi-sphere (Kuzkin 2012)

Idealised flow through deep leg vein

Channel width=12m

ρ_f=1060Kg/m^3

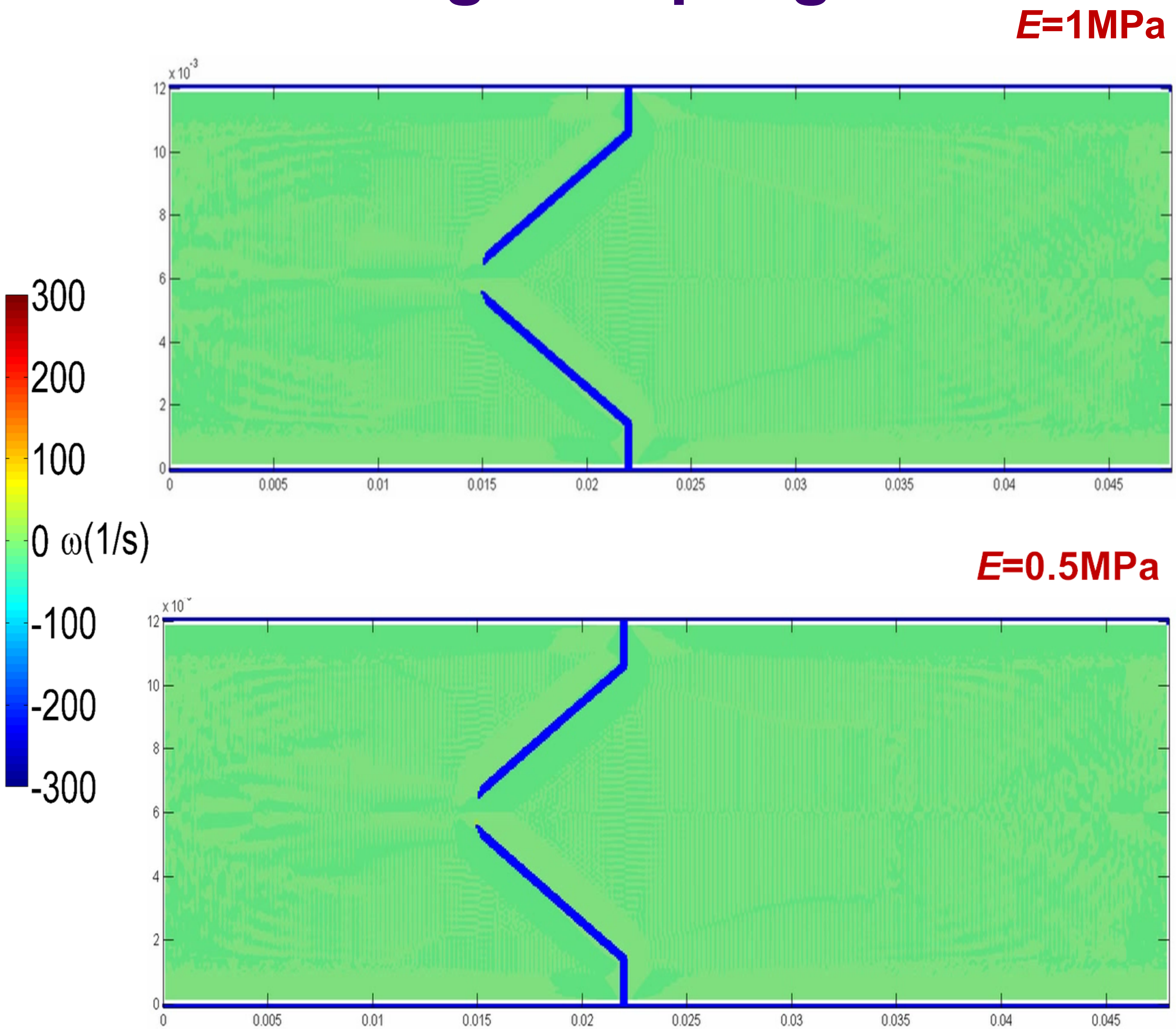
ρ_s=2120Kg/m^3

Valve leaflet

thickness=0.3mm

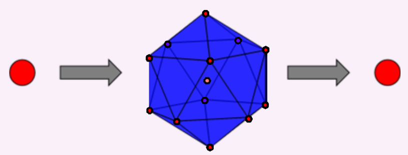
|dP/dx|=2mm(Hg)

Total time=2s



Manchester SPH: New Developments & Possibilities

Development of 3-D dynamic particle refinement SPH on GPUs with U-Vigo & U-Parma using DualSPHysics



DualSPHysics

Development of SPH for **THERMAL HYDRAULIC FLOWS**

Development of SPH for **Non-Newtonian flows**

Development of higher-order convergence SPH

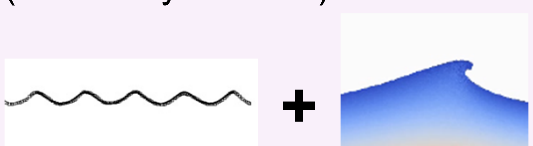
Development of SPH for **Bubbly flows**: intumescent paints & steel production

Development of SPH **Fluid-Structure Interaction (FSI)**

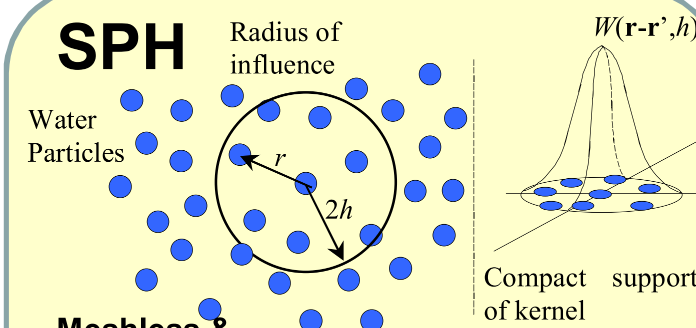
Froude Krylov forces; membranes

Development **COUPLING SPH with a far-field model** with City University

(funded by EPSRC)



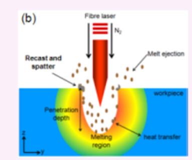
SPH



Meshless & nonlinear simulation technique

$$\langle A(\mathbf{r})\rangle \approx \sum_{j=1}^{N} A_j\, W(\mathbf{r}-\mathbf{r}_j, h)\frac{m_j}{\rho_j}$$

Development of 3-phase laser cleaning & keyhole processing SPH model



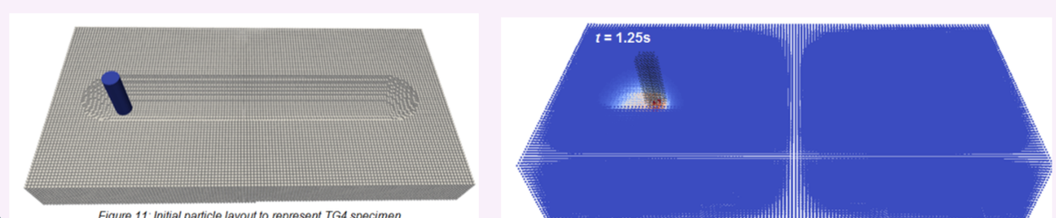
Application to Soil Erosion with University of Brasil for agriculture

(funded by EPSRC)

Development for granular flows and Hot Isostatic Pressing (HIP)

(funded by EPSRC NNUMAN)

Development of **multi-phase SPH for WELDING on GPUs**



Manchester MaSC SPH Group 2016

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Dr Steve Lind

Collaborating Academic Staff

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Prof. Yong Wang

Dr Lee Cunningham

Dr Alistair Revell

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Permanent Visitors

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Alex Chow

Sam Hunter

Annelie Baines

Aaron English

Katy Walton

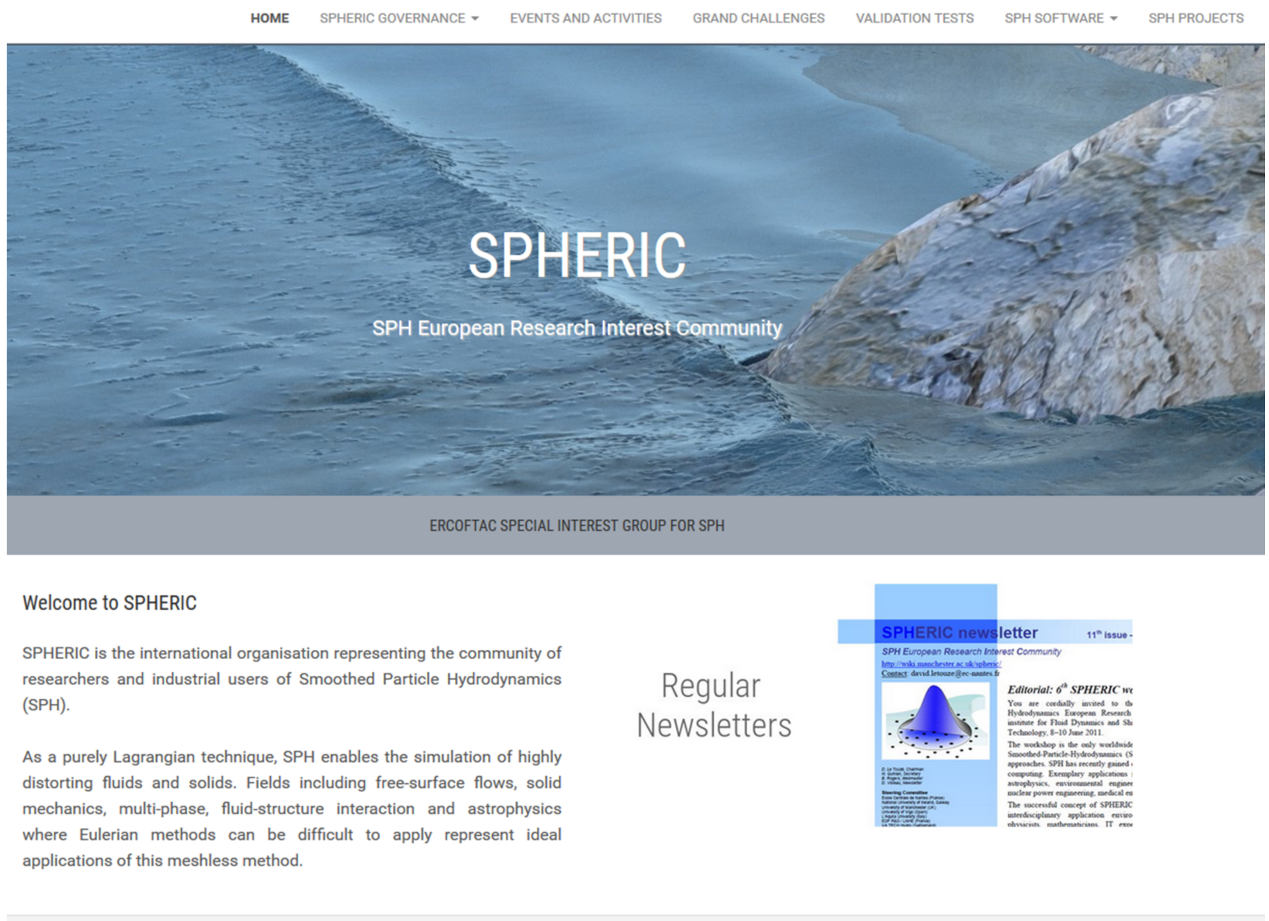
+ 11 PhDs graduated

eDF NATIONAL NUCLEAR LABORATORY Unilever

SPHERIC

International Research Initiative: https://spheric-sph.org

- Founding members
- Steering Committee
- Webmasters
  BDR: 2005-2015
  AJC: 2015 -
- Chair (2015 - 2020)
  - 11 International Workshops
  - **2017 in Ourense**
  - Training Day



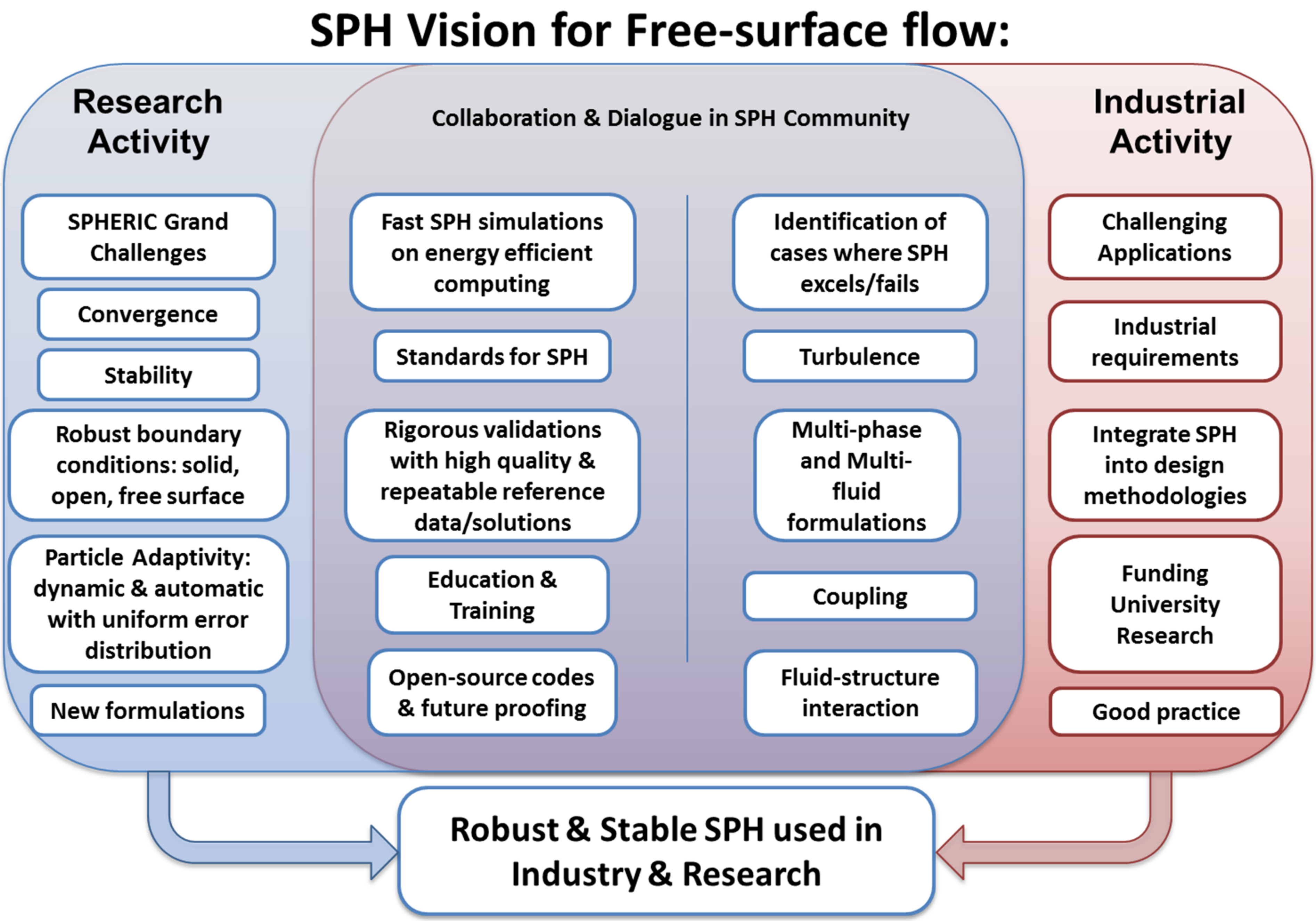
- 75 Institutions are members: universities, government research labs & industrial companies

Key Issues in SPH: SPHERIC Grand Challenges & then some

1. **Convergence and Accuracy** – this is still in development and not proven theoretically (the fully Lagrangian approach currently has a 2nd-order upper bound)
2. **Numerical stability** – this is still unproven
3. **Boundary Conditions** – probably the worst culprit of all problems for free-surface flow
4. **Adaptivity** – efficient simulations are key for engineering application

- **Very small timestep & Formulation** for simulation involving many free-surface wave problems – SPH is good & bad: OTHER METHODS?

- **Turbulence** – a very difficult topic in its own right is yet to receive comprehensive investigation



Violeau & Rogers (2016), “SPH for free-surface flow: past, present and future”, *Journal of Hydraulic Research.*

DualSPHysics Users Workshop

Workshop origins

Workshop structure

MANCHESTER 1824

DualSPHysics Users Workshop

Origins:

- Since release, DualSPHysics has been downloaded 1000s times
- DualSPHysics website has a **users' forum** where a lot of questions get asked about how to use the code.
- We often get approached by both industrial companies & academic organisations who ask us one question repeatedly:

"Can SPH do this?"

Aims of Workshop:

- Hear how other users of DualSPHysics are using the code
- Hear the latest developments from the DualSPHysics team
- Give you an opportunity to make suggestions to help guide the future development of the DualSPHysics project.

DualSPHysics v4 New Features

- Structure of the CPU and GPU code:
- Optimisation of the size of blocks for execution of CUDA kernels:
- Double precision
- Improved formulation for adding external forces
- Movement from external file for rotation
- Coupled SPH & DEM
- Multi-Phase soil-water
- Novel Shifting algorithm
- Automatic wave generation
- More powerful GenCase using OpenMP
- New options in MeasureTool for moving probe points
- Force computation
- More information for floating bodies and motion analysis
- Store information with variable output time
- New properties for different type of fluids or boundaries
- New variables in post-processing tools defined by the user
- Alternative building method via CMAKE (https://cmake.org/)

Thank you

Acknowledgments

- U-Man: Abouzied Nasar, Alex Chow, George Fourtakas, Athanasios Mokos, Gede Pringgana
- U-Vigo: Alex Crespo, Jose Dominguez, Moncho Gomez-Gesteira, Anxo Barreiro
- Flanders Hydraulics: Corrado Altomare
- U-Parma: Renato Vacondio
- U-Lisbon: Ricardo Canelas

Websites

- Free open-source Dual**SPHysics** code:
  http://www.dual.sphysics.org
- **SPHERIC** = SPH European Research Interest Community:
  http://wiki.manchester.ac.uk/spheric